AD NUMBER
AD815185
LIMITATION CHANGES
TO: **Approved for public release; distribution is unlimited.**
FROM: **Distribution authorized to U.S. Gov't. agencies and their contractors; Critical Technology; MAY 1967. Other requests shall be referred to Air Force Weapons Laboratory, Attn: WLRT, Kirtland AFB, NM 87117. This document contains export-controlled technical data.**
AUTHORITY
AFWL ltr, 30 Nov 1971

The following notice applies to any unclassified (including originally classified and now declassified) technical reports released to "qualified U.S. contractors" under the provisions of DoD Directive 5230.25, Withholding of Unclassified Technical Data From Public Disclosure.

NOTICE TO ACCOMPANY THE DISSEMINATION OF EXPORT-CONTROLLED TECHNICAL DATA

1. Export of information contained herein, which includes, in some circumstances, release to foreign nationals within the United States, without first obtaining approval or license from the Department of State for items controlled by the International Traffic in Arms Regulations (ITAR), or the Department of Commerce for items controlled by the Export Administration Regulations (EAR), may constitute a violation of law.

2. Under 22 U.S.C. 2778 the penalty for unlawful export of items or information controlled under the ITAR is up to ten years imprisonment, or a fine of $1,000,000, or both. Under 50 U.S.C., Appendix 2410, the penalty for unlawful export of items or information controlled under the EAR is a fine of up to $1,000,000, or five times the value of the exports, whichever is greater; or for an individual, imprisonment of up to 10 years, or a fine of up to $250,000, or both.

3. In accordance with your certification that establishes you as a "qualified U.S. Contractor", unauthorized dissemination of this information is prohibited and may result in disqualification as a qualified U.S. contractor, and may be considered in determining your eligibility for future contracts with the Department of Defense.

4. The U.S. Government assumes no liability for direct patent infringement, or contributory patent infringement or misuse of technical data.

5. The U.S. Government does not warrant the adequacy, accuracy, currency, or completeness of the technical data.

6. The U.S. Government assumes no liability for loss, damage, or injury resulting from manufacture or use for any purpose of any product, article, system, or material involving reliance upon any or all technical data furnished in response to the request for technical data.

7. If the technical data furnished by the Government will be used for commercial manufacturing or other profit potential, a license for such use may be necessary. Any payments made in support of the request for data do not include or involve any license rights.

8. A copy of this notice shall be provided with any partial or complete reproduction of these data that are provided to qualified U.S. contractors.

DESTRUCTION NOTICE

For classified documents, follow the procedure in DoD 5220.22-M, National Industrial Security Program, Operating Manual, Chapter 5, Section 7, or DoD 5200.1-R, Information Security Program Regulation, Chapter 6, Section 7. For unclassified, limited documents, destroy by any method that will prevent disclosure of contents or reconstruction of the document.

AD815185

NUCLEAR EXPLOSION INTERACTION STUDIES

Volume I

Methods for Analysis of Radiative Transfer

K. D. Pyatt, Jr., et al.

General Atomic Division
General Dynamics Corporation
Special Nuclear Effects Laboratory
San Diego, California

Contract AF 29(601)-7035

TECHNICAL REPORT NO. AFWL-TR-66-108, Vol. I

May 1967

AIR FORCE WEAPONS LABORATORY
Research and Technology Division
Air Force Systems Command
Kirtland Air Force Base
New Mexico

AFWL-TR-66-108, Vol. I

Research and Technology Division
AIR FORCE WEAPONS LABORATORY
Air Force Systems Command
Kirtland Air Force Base
New Mexico

AFWL-TR-66-108, Vol. I

NUCLEAR EXPLOSION INTERACTION STUDIES

Volume I

Methods for Analysis of Radiative Transfer

K. D. Pyatt, Jr., et al.

General Atomic Division
General Dynamics Corporation
Special Nuclear Effects Laboratory
San Diego, California

Contract AF29(601)-7035

TECHNICAL REPORT NO. AFWL-TR-66-108, Vol. I

FOREWORD

This report was prepared by General Atomic Division, General Dynamics Corporation, San Diego, California, under Contract AF29(601)-7035. The research was funded by DASA under Program Element 6.16.46.01D, Project 5710, Subtask 07.002, and by ARPA Order 3[illegible], Program Element 6.?5.03.01.R.

Inclusive dates of research were 22 July 1965 to 21 July 1966. The report was submitted 28 April 1967 by the AFWL Project Officer, Maj George Spillman (WLRT). The contractor's report number is GA-7370.

This final report on Nuclear Explosion Interaction Studies is being published in four volumes. The volume titles are as follows: Volume I, Methods for Analysis of Radiative Transfer; Volume II, Methods for Analysis of Thermal Phenomena; Volume III, Miscellaneous Code Development; and Volume IV, Phenomenology Studies (classified SECRET/RESTRICTED DATA).

The first three volumes are devoted, respectively, to theoretical studies and computer code development in radiative transfer, thermal phenomena, and miscellaneous efforts related to various other aspects of the work. The fourth volume, which is classified, contains the results of applications of these techniques, and of those previously developed, to the study of fireball growth and the interaction of laser radiation with materials.

The NEIS program is long-range, and most of the projects described in this report are in an incomplete state of development. This is due in part to the nature of the existing computer programs themselves, which continue in a state of development as long as they are in use, and in part to the time scale involved in bringing new programs to a state of capability for solving real problems.

General Atomic staff personnel contributing to the research include J.H. Alexander, C.R. Dismukes, R. Durstenfeld, R.S. Engelmore, B.E. Freeman, W.B. Lindley, J.T. Palmer, K.D. Pyatt, L.L. Reed, L.M. Schalit, J.R. Triplett, and numerous others. The cooperation of Col R.H. Pennington, Maj G.R. Spillman, Lt B.S. Chambers, III, Lt N.D. Morgan, Lt R.A. Howerton, Dr. P.V. Avizonis, and Mr. D.W. Lane of the Air Force Weapons Laboratory is gratefully acknowledged.

This report has been reviewed and is approved.

George R. Spillman

GEORGE R. SPILLMAN
Major, USAF
Project Officer

for George R. Spillman

RALPH H. PENNINGTON
Colonel, USAF
Chief, Theoretical Branch

Claude K. Stambaugh

CLAUDE K. STAMBAUGH
Colonel, USAF
Chief, Research Division

ABSTRACT

The non-equilibrium diffusion approximation to the radiative-transfer equation is developed. The first two moments of the radiative transfer equation, including Thomson scattering and pure absorption, are formed, and the equations are closed by a relation between the radiation energy and pressure. Applications of SPUTTER non-equilibrium diffusion subroutines to several simple radiative-transfer problems are described and compared with results from other numerical radiative-transfer codes. Subroutines are also described which calculate the effect of Thomson scattering in TAMALE. The method of moments, the method of discrete ordinates or characteristics, and the Monte Carlo method are described with special reference to the calculation of radiative transport in two dimensions. Their relative merits are discussed, and considerations bearing on the choice of which to use in various applications are given. The non-equilibrium diffusion approximation, which is the variant of the moments method used in DRADTN and ERADTN, has been extended to axially symmetric configurations of two dimensions in a new program, TDRAD. The method of characteristics has been programmed for the same geometry as that treated by TDRAD. The new code, TRAN2, extends TDRAD to situations in which the radiation is too anisotropic to be described by only two moments. The problem of averaging absorption coefficients and scattering cross sections is a basic one in any calculation of radiative transport. A proposed solution is formulated, and transmission functions are derived for the case where opacities may be considered piecewise constant in space and frequency.

(Distribution Limitation Statement No. 2)

This page intentionally left blank.

CONTENTS

I. NON-EQUILIBRIUM DIFFUSION METHODS FOR SPUTTER . . . 1
1.1. Introduction . . . 1
1.2. Differential Equations of Non-equilibrium Diffusion . . . 3
1.3. Difference Equations and Boundary Conditions . . . 7
1.4. How to Use Non-equilibrium Diffusion Subroutines . . . 24
1.5. Test Problems . . . 34
1.6. Appendix: Stability Analysis . . . 41
1.7. Appendix: Listing of ERADTN and DRADTN . . . 49
References . . . 72

II. SCATTERING METHODS FOR TAMALE . . . 73
2.1. Introduction . . . 73
2.2. Analysis of the Transport Equation with Compton Scattering . . . 73
2.3. Numerical Solution of the Transport Equation with Thomson Scattering . . . 77
2.4. The TAMALE Code . . . 79
References . . . 81

III. TWO-DIMENSIONAL RADIATION TRANSPORT TECHNIQUES: A SURVEY OF METHODS . . . 82
3.1. Introduction . . . 82
3.2 The Method of Moments . . . 84
3.3. Discrete Ordinates . . . 87
3.4. The Monte Carlo Method . . . 95
3.5. Conclusions . . . 96
References . . . 98

IV. NON-EQUILIBRIUM DIFFUSION METHODS FOR HECTIC . . . 99
4.1. Introduction . . . 99
4.2. The Finite Difference Approximation . . . 100
4.3. Boundary Conditions . . . 102
4.4. Methods for Solving the System . . . 105
4.5. Procedure for Solving the System . . . 105
4.6. The Subprogram TDRAD . . . 107
4.7. Outline of TDRAD . . . 113
4.8. Review of the Code Development . . . 113
4.9. Appendix: Listing of TDRAD . . . 117

CONTENTS (Continued)

V. THE METHOD OF CHARACTERISTICS IN CYLINDRICAL GEOMETRY 126
5.1. Introduction 126
5.2. The Local Coordinate System 126
5.3. Distribution of Rays 127
5.4. Calculation of Intensities 131
5.5. Thick Zones 132

VI. FREQUENCY-AVERAGED TRANSMISSION FUNCTIONS 134
6.1. Introduction 134
6.2. Frequency Averaging for the Transport Equation 137
6.3. Parametric Representation of Transmission Functions 143
References 146
Distribution 147

Figures

1. Slab Penetration Fluxes 36
2. Slab Penetration Temperature Profiles 37
3. Spherical Emission Test Problem, $\Delta t = 0.03$, $\kappa_R = \kappa_P = 0.2$ 39
4. Spherical Emission Test Problem, $\Delta t = 0.03$, $\kappa_R = \kappa_P = 0.1$ 39
5. Spherical Emission Test Problem, $\Delta t = 0.03$, $\kappa_R = \kappa_P = 0.5$ 40
6. Flux Versus Time for Spherical Emission Test Problem, $t = 0.03$ 40
7. Typical Distribution of Directions 88
8. Typical Short Characteristic 92
9. Hydrodynamic Mesh 100
10. Typical Cell of Mesh 100
11. Configuration of Test Problem 115
12. Coordinate Vectors 127
13. Components of Ω 129
14. Long Characteristic 129
15. Coordinates μ and λ 129

DOCUMENTS PRODUCED UNDER CONTRACT AF 29(601)-7035

Alexander, J. H., "Numerical Methods for Solving Two-Dimensional Problems of Radiative Transport," General Atomic Report GAMD-7047, 1966. (Unclassified)

Freeman, B. E., "Polarization Effects on Radiative Diffusion in a Compton Scattering Medium," General Atomic Report GA-6157, 1966, submitted for publication in Astrophys. J.

Palmer, J. T., "A Comparison of Various Difference Schemes for a Simplified One-Dimensional Transport Equation," General Atomic Report GAMD-6955, 1966. (Unclassified)

"Progress Report for Period Ending September 30, 1965" (U), General Atomic Report GACD-6747(9-65), 1965. (SECRET)

"Progress Report for Period Ending December 31, 1965," General Atomic Report GACD-6747(12-65), 1965. (Unclassified)

"Progress Report for Period Ending March 31, 1966," General Atomic Report GACD-6747(3-66), 1966. (Unclassified)

"Progress Report for Period Ending June 30, 1966," General Atomic Report GACD-6747(6-66), 1966. (Unclassified)

Reed, L. L., "Equation of State Inversion from Temperature-Density to Specific Energy - Density by Table Look-Up," General Atomic Report GAMD-7189 (Rev.), 1966. (Unclassified)

Schalit, L. M., and D. R. Yates, "LPLOT Fortran Program," General Atomic Report GAMD-7104, 1966. (Unclassified)

Teichmann, T., "Numerical Integration on a Sphere," General Atomic Report GAMD-6981, 1966. (Unclassified)

Triplett, J. R., "Heating of a Slab by a Time-Dependent Source," General Atomic Report GAMD-6665, 1965. (Unclassified)

This page intentionally left blank.

SECTION I

NONEQUILIBRIUM DIFFUSION METHODS FOR SPUTTER

1.1. INTRODUCTION

Solutions of the radiation transport equation are required in a substantial number of problems involving the transport of energy in high-temperature gases. In this report, numerical solutions to some sample problems are obtained by a method known as the non-equilibrium diffusion approximation. Comparison with numerical solutions gives an indication of the usefulness of the method.

An explicit formulation of the non-equilibrium diffusion equations for slab geometry and pure absorption has been tested (Ref. 1)* and found to constitute a useful approximation to slab penetration problems in the grey atmosphere approximation. Additional tests of the time independent diffusion equations have been made (Ref. 2) by comparison with transport solutions of Milne problems. Independently, the differential non-equilibrium diffusion equations have been derived for the case of radiation interaction through Compton scattering (Ref. 3). The possibility of using the Rosseland and Planck mean opacities, of performing multigroup calculations, and of formulating the difference equations in partially implicit and fully implicit (unconditionally stable) forms has also been noted (Ref. 4). Consequently, the method can be expected to provide generally applicable approximate equations that can be solved economically for one-dimensional geometries and ultimately two-dimensional geometries.

In this report, derivation of the differential equations is presented (Section 1.2), and then these equations are formulated in difference form (Section 1.3) for the one-dimensional geometries (slabs, cylinders, spheres). The code has been incorporated as a subroutine into the SPUTTER code, a one-dimensional, radiation transport — hydrodynamics

*References appear at the end of each section.

code applicable to many high-energy flow phenomena. The subroutine can perform either grey or multifrequency group problems and contains options for determining whether partially or fully implicit equations are solved. The nonlinear coefficients of the equations may be formed more accurately by exercising the option to iterate the equations to time-center the coefficients. At the outside boundaries of the mesh, the following options can be selected: (1) zero net flux (reflection), (2) zero backward current (vacuum), and (3) prescribed backward current (frequently the blackbody boundary condition). Two versions of the code are available as separate subroutines. The DRADTN subroutine (see Section 1.7 for the FORTRAN listing) includes the effects of radiation retardation (energy stored in the radiation field and the propagation of light waves), and is particularly applicable to problems involving temperatures in the kev range, where temperature waves propagate at near light speed. For problems involving temperatures in the ev range, in which changes are slow compared with the light speed, a more economical and accurate code is the ERADTN version (see Section 1.7 for the FORTRAN listing), which omits the retardation terms.

In Section 1.4, features of the codes of special interest to the user are discussed. A glossary of terms appearing in the code is also presented in that section, and particular attention is given to the quantities which must be supplied to control the code. Values for the control quantities are recommended, and the effects of deviations from them are discussed.

In the slab and spherical geometry, radiation transport subroutines for SPUTTER are available (Ref. 5). Two of these subroutines, called PRADTN (for plane radiation) and SRADTN (for spherical radiation), have been used to perform a series of test problems (see Section 1.5) having relatively simple initial conditions and material properties. Comparison with the solution of the corresponding problem using DRADTN and ERADTN indicates the error to be expected when similar problems are calculated.

An attempt is made to isolate the effects of the form of the difference equations from the different treatments of the frequency dependence.

1.2. DIFFERENTIAL EQUATIONS OF NON-EQUILIBRIUM DIFFUSION

The equations of non-equilibrium diffusion are the first two moment equations of the radiation transport equation. In this section, these equations are derived independently of the coordinate system. They are thus applicable to two- and three-dimensional radiation flow problems, but will be specialized to the one-dimensional geometries.

The point of departure is the radiation transport equation for the intensity I at position $\vec{r}$ at time t in the direction specified by the unit vector $\vec{\Omega}$. Interaction of the radiation with the material is characterized by the coefficient for pure absorption μ_a and the scattering coefficient μ_s. When the source function is approximated by the local thermodynamic equilibrium assumption in terms of the Planck function B, and scattering is given by the Thomson limit of the Compton cross section, the transport equation is as follows:

$$\frac{1}{c}\frac{\partial I}{\partial t} + \vec{\Omega} \cdot \nabla I = \mu_a (B - I) - \mu_s I + \frac{3\mu_s}{16\pi}\int d\Omega' \left[1 + (\vec{\Omega} \cdot \vec{\Omega}')^2\right] I' \qquad (1)$$

where I' is the intensity in the direction $\vec{\Omega}'$. The frequency dependence has been suppressed, since in the Thomson limit in which scattering occurs without frequency shift, Eq. (1) applies to a single frequency. The polarization of the photons has also been neglected by averaging the scattering integral over polarization in the supposedly unpolarized incident beam.

On the boundaries of the system, the transport equation must be supplemented with a specification of the intensity of all rays passing through the boundary from outside to inside. That is, $I(\vec{\Omega}) = I_o$ if $\vec{\Omega} \cdot \vec{N} < 0$, where $\vec{N}$ is a vector normal to the surface directed outward.

Moments of the radiation intensity are obtained by integrating powers of $\vec{\Omega}$ over the entire solid angle. The radiation energy scalar E, the

approximation employed above depends on temperature only through the density of free electrons,

$$\mu_s = \frac{8\pi}{3} r_o^2 N_e \ (\mathrm{cm}^{-1})$$

where r_o is the classical electron radius (= 2.8×10^{-13} cm) and N_e is the free electron density (cm^{-3}). In practice, μ_s is negligible compared with μ_a if temperatures are not sufficiently large to produce substantially complete ionization. Consequently, the assumption of the temperature independence of μ_s is an excellent approximation. Changes in material temperature are assumed to take place under the combined effects of radiation absorption or emission, hydrodynamic motions of the material, and energetic sources within the material.

1.3. DIFFERENCE EQUATIONS AND BOUNDARY CONDITIONS

By specializing the equations given in Section 1.2 to one spatial dimension, the one-dimensional non-equilibrium diffusion equations are obtained:

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial r^{\alpha}} (\alpha r^{\alpha - 1} F) = c \mu_a (4\pi B - E)$$

$$\frac{1}{c} \frac{\partial F}{\partial t} + \frac{c}{3} \frac{\partial E}{\partial r} = - \frac{F}{\lambda} \tag{10}$$

where the geometry coefficient α takes the value 1, 2, or 3, corresponding to slab, cylinder, or sphere, respectively.

1.3.1. Spatial Difference Equations

These equations are to be replaced by approximating difference equations in a way dictated by accuracy, stability, and ease of computing. The quantities in Eq. (10) are associated with zonal boundaries or interiors as suggested by an integration of the first equation over the zone. The resulting equation describing the conservation of energy is given by

$$\frac{\partial E_{i+1/2}}{\partial t} + \frac{1}{r_{i+1}^{\alpha} - r_i^{\alpha}} (\tilde{F}_{i+1} - \tilde{F}_i) = c\,(\mu'_a)_{i+1/2} (4\pi B_{i+1/2} - E_{i+1/2}) \quad (11)$$

where $\tilde{F}_i = \alpha\, r_i^{\alpha-1}\, F_i$, corresponds to the flux at the i^{th} zone boundary integrated over the surface area. Difference equation (11) is formulated in a conservative fashion; i. e., radiation flux out of one zone enters the neighboring zone undiminished. The quantities with half-integral subscripts, $E_{i+1/2}$ and $B_{i+1/2}$, are averages over the zone and are weighted by the zone volume. The second equation for the interface flux is obtained by approximating the derivative by a centered difference

$$\frac{1}{c} \frac{\partial \tilde{F}_i}{\partial t} + \frac{2c}{3}\, \alpha\, r_i^{\alpha-1} \frac{\left(E_{i+1/2} - E_{i-1/2}\right)}{r_{i+1} - r_{i-1}} = - \frac{\tilde{F}_i}{\lambda_i} \quad (12)$$

The material internal energy E_m (erg/g) is taken to be a zone-centered quantity to retain the centering of the third equation,

$$\frac{d\,(E_m)_{i+1/2}}{dt} = - \frac{c}{\rho} \int_0^{\infty} d\nu\, (\mu'_a)_{i+1/2} (4\pi B_{i+1/2} - E_{i+1/2}) - P \frac{d\tau}{dt} + q \quad (13)$$

This equation contains the pressure P, the specific volume τ, the density ρ, and the source q (erg/g sec).

Since the right-hand terms of Eqs. (11) and (13) represent the coupling between radiation and material energies, it is important, in order to ensure energy conservation, that the identical form be used in each equation. Through the equation of state, the material temperature of the zone is related to the internal energy. In turn, the Planck function B and absorption coefficient μ'_a (being zone quantities) are evaluated as functions of the zone temperature. The mean free path λ (an interface quantity) must be obtained by interpolation between the adjacent zonal quantities.

1.3.2. Temporal Difference Equations

The form of the difference equations in time has far-reaching effects on the stability and ease of numerical solution of the system, as well as on its accuracy. Related to the accuracy of solution are considerations of smoothness of the solution in time (avoidance of bounded but slightly damped oscillations) and positivity of the radiation energy. In view of the importance of the time dependence, several alternatives have been tested, and options for some of them are provided in the subroutines.

One of the most important choices is governed by the physical regime in which the problem lies. The equations are substantially simplified and their centering is changed when the time dependent terms of Eqs. (11) and (12) can be neglected, which corresponds to omitting the $\partial I/\partial t$ term of the transport equation. The equations are sufficiently different that separate subroutines have been written. The ERADTN subroutine (see Section 1.7) contains the code without retardation, in a form applicable to problems in which the radiation energy is considerably smaller than the material energy and in which the light propagation is unimportant. The DRADTN subroutine (see Section 1.7) includes the retardation effects.

The equations for the radiation energy E in both of these codes have the form of linear equations, in each of which three neighboring zones are represented. These simultaneous equations can be solved by a well-known algorithm (Ref. 7) with very little labor. The stability of the resulting equations depends, however, on whether Eq. (13), the material energy equation, has been solved simultaneously with the two equations for the radiation quantities. In turn, the feasibility of obtaining a fully implicit system of equations depends on whether the grey approximation is made or several frequency groups are evaluated. In the latter case, partially implicit equations are obtained with an associated stability restriction (see Section 1.7). The fully implicit equations are presumed to be unconditionally stable.

The distinction between these two cases will be made more precise when the equations are formulated in the next section. These equations are nonlinear through the dependence of absorption coefficients and source functions on temperature.

Since the method of solution outlined above requires a linearization of the equations, the time dependence of the coefficients is not taken into account within the time interval of one time cycle. To improve the accuracy, an iteration may be performed in which the estimate of the temperature change in the first step of the calculation is used to re-evaluate the coefficients for a second calculational step. Further iterations of this cycle are not desirable since second order accuracy is obtained in the first iteration (Ref. 8). In Section 1.3.3 the equations discussed above are presented in detail. The ERADTN equations are given first in both the partially implicit and fully implicit forms. The steps required for iteration are also discussed. The same format is then followed for the DRADTN equations.

1.3.3. Difference Equations for ERADTN (No Retardation)

Without retardation terms, Eqs. (11) and (12) can be written at a particular time instant. Denoting the index of the time by superscript n, where $t^n = \Sigma \Delta t^n$, the first two equations are centered in time at $t^{n+1/2}$, the midpoint of the interval, $\Delta t^n = t^{n+1} - t^n$:

$$P_i (\tilde{F}^{n+1/2}_{i+1} - \tilde{F}^{n+1/2}_{i}) = c\,\mu_i\,(b_j \varphi_i - E^{n+1/2}_i)$$

$$R_i (E^{n+1/2}_i - E^{n+1/2}_{i-1}) - \frac{\tilde{F}^{n+1/2}_i}{4\lambda_i} \tag{14}$$

where $P_i = 1/(r^{\alpha}_{i+1} - r^{\alpha}_i)$, $\varphi_i = a\,\theta^4_i$, and $R_i = c\alpha r^{\alpha-1}_i/6(r_{i+1} - r_{i-1})$. In the above equations spatial indices have all been made integral by subtracting 1/2 from the half-integral indices. This is the same convention as is

practiced in the SPUTTER code. The source function and coefficients depend on temperature and, for accuracy, should be evaluated as a function of $\theta_i^{n+1/2}$, the temperature at $t^{n+1/2}$.

The frequency dependence has been suppressed except in the source term. Equations (14) result from integration over frequency groups. As is discussed more fully in Section 1.4, absorption coefficients are averaged over the frequency interval, and the source function is

$$\int_{\nu_j}^{\nu_{j+1}} 4\pi B d\nu = b_j \varphi_i$$

where b_j is the normalized partial Planck function.

1.3.4. Partially Implicit Equations for ERADTN

In the partially implicit solution, the two equations (14) are solved for E and F with the source function and coefficients considered as known quantities. Since in this approximation the equations are linear with non-zero values for three neighboring terms, the equations for E become (suppressing time indices):

$$A_i E_{i-1} + B_i E_i + C_i E_{i+1} + D_i = 0 \tag{15}$$

where

$$\begin{aligned} A_i &= -4\lambda_i R_i P_i \\ C_i &= -4\lambda_{i+1} R_{i+1} P_i \\ B_i &= c\mu_i - A_i - C_i \\ D_i &= -c\mu_i b_j \varphi_i \end{aligned} \tag{16}$$

The energy equation (13) can be solved for the temperature change using the equation of state

$$\frac{d\theta_i}{dt} = \left(\frac{dE_m}{dt} - \frac{\partial E_m}{\partial \tau}\frac{d\tau}{dt}\right)/C_v \tag{17}$$

where the specific heat C_v (ergs/(g ev)) has been introduced, to obtain

$$\theta_i^{n+1} = \theta_i^n + \frac{\Delta t^n}{(C_v)_i}\left[q_i - \left(P_i + \frac{\partial E_m}{\partial \tau}\right)\frac{d\tau}{dt} - \frac{c}{\rho}\sum_j \mu_{ij}\left(b_j \varphi_i - E_{ij}^{n+1/2}\right)\right] \tag{18}$$

In Eq. (18) the frequency dependence of the source function is denoted by the index j, which stands for a partitioning of the spectrum into frequency groups.

The order of the solution of these equations is as follows: First, Eq. (16) for the coefficients is evaluated as a function of θ_i^n; second, Eq. (15) is solved for $E_i^{n+1/2}$ for all frequency groups (see Section 1.7); third, Eq. (18) is used to find θ_i^{n+1}. In the event that rapid changes of temperature occur or the coefficients depend strongly on temperature, an iteration can be performed. The centered temperature is estimated to be $\theta^{n+1/2} = (\theta^n + \theta^{n+1})/2$, which is used to re-evaluate Eq. (16). The second and third steps of the calculation are repeated as above. The iteration is terminated after the second pass.

The partially implicit equations can be employed for the grey atmosphere (one frequency group) approximation but are generally inferior to the method discussed below. For the multigroup approximation, however, they are required.

1.3.5. Fully Implicit Equations for ERADTN

For a single frequency group ($b_j = 1$), it is possible to solve simultaneously for the temperature from Eq. (18) and the radiation energy. This is desirable because the stability condition required by the partially implicit equations can thereby be relaxed. First, it is necessary to

linearize Eq. (18). Since $a\theta_i^4 \equiv \varphi_i$ appears in Eq. (14), it is also chosen for the linearization variable of Eq. (18):

$$\varphi_i^{n+1} = \varphi_i^n + \frac{4a\theta_i^3 \Delta t^n}{(C_v)_i}\left[q_i - \left(P_i + \frac{\partial E_m}{\partial \tau}\right)\frac{d\tau}{dt} - \frac{c\mu_i}{2\rho}\left(\varphi_i^{n+1} + \varphi_i^n - 2E_i^{n+1/2}\right)\right] \tag{19}$$

Second, the first equation of Eqs. (14) is rewritten to maintain the parallelism between the energy exchange terms and to introduce φ_i^{n+1}:

$$P_i\left(\tilde{F}_{i+1}^{n+1/2} - \tilde{F}_i^{n+1/2}\right) = \frac{c\mu_i}{2}\left(\varphi_i^{n+1} + \varphi_i^n - 2E_i^{n+1/2}\right) \tag{20}$$

By substituting for $\tilde{F}^{n+1/2}$ and φ^{n+1}, an equation of the form of Eq. (15) is is obtained in which

$$A_i = -4\lambda_i R_i P_i, \qquad C_i = -4\lambda_{i+1} R_{i+1} P_i$$

$$B_i = A_i - C_i + \cfrac{1}{\cfrac{1}{c\mu_i} + \cfrac{2a\theta_i^3 \Delta t^n}{\rho (C_v)_i}} \tag{21}$$

$$D_i = \frac{\left[\left(P_i + \frac{\partial E_m}{\partial \tau}\right)\rho\frac{d\tau}{dt} - \rho q_i\right]\frac{2a\theta_i^3 \Delta t^n}{\rho (C_v)_i} - \varphi_i^n}{\frac{1}{c\mu_i} + \frac{2a\theta_i^3 \Delta t^n}{\rho (C_v)_i}}$$

Solution of the fully implicit equations requires evaluation of the coefficients as functions of θ^n in Eq. (21) and the radiation energies in Eq. (15). The temperature is obtained last (Eq. (19)) and can be used for improving the accuracy of solution by iteration. An estimate of the centered temperature $\theta^{n+1/2} = (\theta^n + \theta^{n+1})/2$ is used to evaluate the coefficients a second time; then a second evaluation of the radiation energies is performed. Since the time dependence of the source term is taken more fully into account in the fully implicit equations than in the partially implicit ones,

the former should be more accurate. Hence, for grey problems there appear to be no reasons (aside from code intercomparisons) for performing partially implicit calculations.

1.3.6. Difference Equations for DRADTN (Retardation Included)

The spatial dependence of the DRADTN equations remains the same as for the ERADTN equations, i.e., as given by Eqs. (11) and (12). However, retention of the time derivative terms in the moment equations imposes additional requirements on the difference equations. First, the possibility of instabilities associated with the streaming of radiation and with the exchange of radiation energy and material energy requires care in formulating the difference equations. Even stable difference forms may be undesirable due to small damping of oscillations. Second, the occurrence of $\partial E/\partial t$ and $\partial F/\partial t$ in Eq. (10) suggests that, in order to center the equations at $t^{n+1/2}$, quantities at $t^n(E^n, F^n)$ be introduced. With them, first differences in time centered at $t^{n+1/2}$ can be formed. Third, the consideration of the conservation of energy must now take account of the radiation energy. As is the case for the ERADTN equations, it is highly desirable that a difference analogue of total energy be conserved exactly by the DRADTN equations.

With centered first differences in time for the first derivatives introduced in Eqs. (11) and (12), the DRADTN equations corresponding to Eq. (14) are given by

$$\frac{E_i^{n+1} - E_i^n}{\Delta t^n} + \frac{P_i}{2}\left(\tilde{F}_{i+1}^{n+1} - \tilde{F}_i^{n+1} + \tilde{F}_{i+1}^n - \tilde{F}_i^n\right) = \frac{c\mu_i}{2}(2b_j\varphi_i - E_i^{n+1} - E_i^n)$$

$$\frac{\tilde{F}_i^{n+1} - \tilde{F}_i^n}{c\Delta t^n} + 2R_i\,(E_i^{n+1} - E_{i-1}^{n+1} + E_i^n - E_{i-1}^n) = -\frac{\tilde{F}_i^{n+1} + \tilde{F}_i^n}{2\lambda_i} \tag{22}$$

These equations employ the definitions following Eq. (14). Equations (22) have the following properties: (1) they are linear in E and F for ease in

solution, (2) they are centered at $t^{n+1/2}$ for accuracy, (3) they conserve energy in the sense discussed above, and (4) they are expected to be stable against oscillations of the radiation field.

These equations, which are further analyzed below, were the first equations to be coded. As noted in Section 1.6, their solutions are subject to oscillations which, in some cases, are very slightly damped. The equations currently in use are discussed later in this section.

1.3.7. Partially Implicit Equations for DRADTN

For multifrequency problems and as an option for grey problems, the partially implicit form of the equations is solved. In these equations, the source function and the coefficients are evaluated from the available temperatures, θ_i^n. When solved for the unknown quantities E_i^{n+1}, Eqs. (22) again have the form of Eq. (15), in which the coefficients are

$$A_i = -Q_i R_i P_i$$

$$C_i = -Q_{i+1} R_{i+1} P_i$$

$$B_i = \frac{1}{\Delta t^n} - A_i - C_i + \frac{c\mu_i}{2} \tag{23}$$

$$D_i = \left(-\frac{1}{\Delta t^n} + \frac{c\mu_i}{2}\right) E_i^n + A_i \left(E_{i-1}^n - E_i^n\right) + C_i \left(E_{i+1}^n - E_i^n\right)$$

$$+ \frac{P_i}{c\Delta t^n} \left(Q_{i+1} \tilde{F}_{i+1}^n - Q_i \tilde{F}_i^n\right) - c\mu_i b_j \varphi_i$$

where

$$Q_i = \frac{1}{\dfrac{1}{c\Delta t^n} + \dfrac{1}{2\lambda_i}} .$$

The partially implicit formulation makes use of E_i^{n+1} obtained above in an energy equation similar to Eq. (18). By using Eq. (17), but paralleling the formulation of the radiation-material exchange term of Eq. (22), the equation for the new temperature becomes

$$\theta_i^{n+1} = \theta_i^n + \frac{\Delta t^n}{(C_v)_i}\left[q_i - \left(P_i + \frac{\partial E_m}{\partial \tau}\right)\frac{d\tau}{dt} - \frac{c}{2\rho}\sum_j \mu_{ij}(2b_j\varphi_i - E_{ij}^n - E_{ij}^{n+1})\right] \quad (24)$$

As in the case of the ERADTN equations, an iteration may be performed in which the equations are solved a second time using coefficients formed with $\theta^{n+1/2} = (\theta^n + \theta^{n+1})/2$.

1.3.8. Fully Implicit Equations for DRADTN

When the grey atmosphere approximation is suitable, the coupling between radiation and material can be made implicit, thereby relaxing the associated stability condition. The energy equation linearized in φ and the zeroth moment equation are similar to Eqs. (19) and (20).

$$\varphi_i^{n+1} = \varphi_i^n + \frac{4a\theta_i^3\Delta t^n}{(C_v)_i}\left[q_i - \left(P_i + \frac{\partial E_m}{\partial \tau}\right)\frac{d\tau}{dt} - \frac{c\mu_i}{2\rho}\left(\varphi_i^{n+1} + \varphi_i^n - E_i^{n+1} - E_i^n\right)\right] \quad (25)$$

$$\frac{E_i^{n+1} - E_i^n}{\Delta t^n} + \frac{P_i}{2}(\tilde{F}_{i+1}^{n+1} - \tilde{F}_i^n + \tilde{F}_{i+1}^n - \tilde{F}_i^n) = \frac{c\mu_i}{2}(\varphi_i^{n+1} + \varphi_i^n - E_i^{n+1} - E_i^n)$$

The coefficients of Eq. (15) are then

$$A_i = -Q_i R_i P_i$$

$$C_i = -Q_{i+1} R_{i+1} P_i$$

$$B_i = -A_i - C_i + \frac{1}{\dfrac{2}{c\mu_i} + \dfrac{4a\theta_i^3 \Delta t^n}{\rho (C_v)_i}} \tag{26}$$

$$D_i = \left(-\frac{1}{\Delta t^n} + \frac{1}{\dfrac{2}{c\mu_i} + \dfrac{4a\theta_i^3 \Delta t^n}{\rho (C_v)_i}} \right) E_i^n + A_i (E_{i-1}^n - E_i^n) + C_i (E_{i+1}^n - E_i^n)$$

$$+ \frac{P_i}{c\Delta t^n} (Q_{i+1} \tilde{F}_{i+1}^n - Q_i \tilde{F}_i^n) - \frac{\varphi_i^n + \dfrac{2a\theta_i^3 \Delta t^n}{(C_v)_i} \left| q_i - \left(P_i + \dfrac{\partial E_m}{\partial \tau} \right) \dfrac{d\tau}{dt} \right|}{\dfrac{1}{c\mu_i} + \dfrac{2a\theta_i^3 \Delta t^n}{\rho (C_v)_i}}$$

If desired Eq. (25) can be solved for the temperature θ^{n+1} to perform an iteration of the implicit equations.

1. 3. 9. Modified DRADTN Equations

The difference equations of Eq. (22), although accurate to second order in time and stable, are subject to oscillations which under some circumstances are very slightly damped, as shown in Section 1. 6. The equations were reformulated in order to remedy these oscillations, which arise from the centering of terms in time and are manifested by periodic exchange of energy between radiation field and material when the time interval greatly exceeds the characteristic relaxation time of the radiation field.

After several experiments, the equations were written in the following form:

$$\frac{E_i^{n+1} - E_i^n}{\Delta t^n} + P_i \left(\tilde{F}_{i+1}^{n+1} - \tilde{F}_i^{n+1} \right) = \frac{c\mu_i}{2} \left(2b_j \varphi_i - 2E_i^{n+1} \right)$$

$$\frac{\tilde{F}_i^{n+1} - \tilde{F}_i^n}{4c\Delta t^n} + R_i \left(E_i^{n+1} - E_{i-1}^{n+1} \right) = - \frac{\tilde{F}_i^{n+1}}{4\lambda_i} \tag{27}$$

These equations have overcome the oscillation difficulties at the expense of loss in accuracy. It is likely that further experimentation in the form of these equations is warranted. In particular, the equations might take the more accurate, centered form in regions where oscillation cannot occur; but in regions where oscillations are possible, the modified equations could be employed.

1.3.10. Boundary Conditions for Difference Equations

The computation in the above equations is assumed to apply to a finite interval, $r_1 \leq r \leq r_I$, at the ends of which boundary currents F_R and F_L are specified as in Eq. (8). These, in turn, relate the flux and energy at the boundary. The difference equations, however, call only for a boundary flux; the radiation energy is a zone centered quantity at best a half zone removed from the surface. It is proposed to close these equations by performing an extrapolation so that the radiation energy at the boundary introduced by Eq. (9) is related to the interior values of energy. The system of equations can then be solved for the energy by the tri-diagonal matrix inversion algorithm.

For illustration, the left boundary condition is derived. It is assumed, just for the purpose of extrapolating the radiation energy through a half zone, that the geometry is planar, that the solution is time independent, and that the source is constant in the half space to the right of x = 0. Then the moment equations can be combined to give

$$\frac{\lambda}{3}\frac{d^2E}{dx^2} - \mu(E - a\theta^4) = 0$$

having the solution $E = a\theta^4 + Ae^{-\alpha x}$, where $\alpha = \sqrt{3\mu/\lambda}$. To determine the constant A, the boundary condition,

$$F(x=0) = 2F_R - E(x=0) = -\frac{\lambda c}{3}\frac{\partial E}{\partial x}\Big)_{x=0}$$

is imposed. The solution,

$$E = a\theta^4 + \frac{2F_R - \frac{ca}{2}\theta^4}{\frac{c\lambda\alpha}{3} + \frac{c}{2}} e^{-\alpha x}$$

gives a boundary flux of

$$F(x=0) = \frac{F_R - \frac{ca}{4}\theta^4}{\frac{3}{4\lambda\alpha} + \frac{1}{2}}$$

The correct solution, giving $F(x = 0) = F_R - (ca/4)\theta^4$, is obtained if $2\lambda\alpha/3 = 1$; consequently, to improve the accuracy of the boundary condition, this substitution is also made in E:

$$E = a\theta^4 + \left(\frac{2}{c}F_R - \frac{a}{2}\theta^4\right)e^{-\alpha x}$$

In order to relate the energy at the boundary E(x = 0) to the energy at the first zone center E_1, the source is eliminated:

$$E(x=0) = \frac{\frac{4}{c}F_R(1 - e^{-\alpha\Delta x_1/2}) + E_1}{2 - e^{-\alpha\Delta x_1/2}}$$

The corresponding value of the boundary flux is

$$F(x=0) = \left(2F_R - \frac{c}{2}E_1\right)\beta_R \tag{28}$$

in which $\beta_R = \frac{1}{2-e^{-\alpha\Delta x_1/2}}$ and $\alpha = \sqrt{3\mu/\lambda}$. For the right-hand boundary the condition is similar:

$$F(x_I) = \left(-2F_L + \frac{c}{2} E_{I-1}\right)\beta_L \tag{29}$$

where $\beta_L = 1/(2 - e^{-\alpha\Delta x_{I-1}/2})$

In Eq. (28), the thickness of the first zone is $\Delta x_1 = r_2 - r_1$ and the quantity α is evaluated as a function of temperature and density in the first zone. Similarly in Eq. (29), for the right-hand boundary condition the last zone thickness is $\Delta x_{I-1} = r_I - r_{I-1}$, the last zone energy is E_{I-1}, and the quantity α is evaluated from the last zone variables.

The expressions for flux at the boundary, Eqs. (28) and (29), after correction for geometry factors,are to be substituted into the zeroth moment equation. The result is a modification of the coefficients of Eq. (15), the linear equation for the unknown radiation energy densities. At the left-hand boundary i = 1, for example, the coefficient $A_1 = 0$, as must be the case to terminate the equations. In addition, the coefficients B_1 and D_1 are modified in a way depending on which form of the equations is being used. To illustrate, the ERADTN coefficients become

$$\begin{aligned} &B_1 + \frac{c}{2}\alpha r_1^{\alpha-1} P_1\beta_R \rightarrow B_1, \\ &D_1 - 2\alpha r_1^{\alpha-1} P_1 F_R \beta_R \rightarrow D_1 \end{aligned} \tag{30}$$

The boundary equations for DRADTN, as currently formulated, are the same as Eq. (30).

1.3.11. <u>Iteration</u>

The coefficients of the linear equations depend on the temperature and, consequently (in a time dependent problem), on the time. In each of

the subroutines an option is provided to use the estimate of the temperature resulting from the first calculation to recalculate the coefficients. The calculation is then repeated. In principle, this iteration could be repeated until a convergence criterion is satisfied. However, the equations are at best no more than second order accurate. Since a single iteration is sufficient to achieve second order accuracy, it is doubtful that further iteration is warranted. Improved accuracy can be better achieved by a reduced time step. The modified DRADTN equations are only first order accurate in time. Consequently, it is doubtful that the iteration option should be exercised for the DRADTN equations.

1.3.12. Solution of E - equations

The equations for the radiation energy at the advanced time, Eqs. (15), form a set of linear equations in which the coefficient matrix of the E-vector is tridiagonal. These equations are solved by factoring the coefficient matrix into upper and lower matrices. The solution is obtained by solving a recurrence relation

$$E_i = g_i E_{i+1} + h_i \tag{31}$$

in which $g_I = 0$ (resulting from $C_I = 0$) and $g_i = -C_i/d_i$, $h_i = -(D_i + A_i h_{i-1})/d_i$, and $d_i = B_i + A_i g_{i-1}$. The condition $A_I = 0$ suffices to terminate the equations for h_1 and d_1.

These equations have been found to suffer from figure loss when the mean free path in the medium is long. To avoid this loss of figures due to the finite precision of the computer, new quantities are defined:

$$\begin{aligned} &A_i' = A_i, \quad C_i' = C_i, \quad D_i' = D_i \\ &B_i' = B_i + A_i + C_i; \; g_i' = g_i - 1 . \end{aligned} \tag{32}$$

In terms of these quantities, the above equations can be written

$$E_i = E_{i+1}(g_i' + 1.) + h_i ,$$

$$g_i' = (-B_i' - A_i g_i')/d_i , \qquad h_i = -(D_i + A_i h_{i-1})/d_i \tag{33}$$

$$d_i = B_i' - C_i + A_i g_i' , \qquad g_I' = -1$$

The modified B_i' is a small quantity when the mean free path is long. The previous equations required the subtraction of the large quantities A_i and C_i from B_i to give the correct result. In addition, under the above circumstances the modified g_i' becomes very small, a result previously achieved by subtraction of quantities near 1 in size.

The flux calculation can also suffer from figure loss. The form of the relation between flux and radiation energy, which is solved for the flux after the radiation energy has been obtained, is given by the first moment equation and is different for DRADTN and ERADTN. Without retardation the result, derived from Eq. (14), is

$$\tilde{F}_i^{n+1} = 4\lambda_i R_i \left(E_{i-1}^{n+1/2} - E_i^{n+1/2}\right) \tag{34}$$

To avoid the subtraction, the flux equation is rewritten

$$\tilde{F}_i^{n+1} = 4\lambda_i R_i \left(h_{i-1} + g_{i-1}' E_i^{n+1/2}\right)$$

Some problems involving temperatures of several kev resulted in overflow of quantities in the fully implicit equations. This overflow was eliminated by forming intermediate quantities in different order, albeit at the cost of less efficient coding.

1.3.13. Time Interval

The control of the time interval reflects two considerations: accuracy and stability. The accuracy criterion is based on limiting the radiation contribution to the energy change in each zone to less than a prescribed fraction of the energy in the zone:

$$\Delta t_R \leq \left(\min_i \frac{E_i}{ER_i}\right) * \text{SLUG} \tag{35}$$

where E_i is the zone internal energy, ER_i is the radiation energy change rate per zone, and the input quantity controlling the accuracy criterion is SLUG. In order to avoid control of the time interval by zones having very small internal energy, the test of Eq. (35) is applied only to zones having greater than a prescribed fraction (given by the input quantity TELM (37)) of the total internal energy.

For problems in which the fully implicit equations are solved, the accuracy criterion affords the only radiative control of the time interval. When the partially implicit equations are solved, however, additional stability criteria are required. The full equations have not yet been subjected to stability analysis. However, the stability analyses given in

Section 1.6 suggest that two criteria be applied. These two conditions must be observed in order that small oscillations will not be amplified when energy is exchanged between radiation and material. The first condition represents stability in the exchange in a single zone between radiation and material:

$$\Delta t_R \leq \min_i \frac{(C_v)_i}{8 \times 10^{12} \theta_i^3 (\kappa_p)_i} \tag{36}$$

where the Planck mean opacity κ_p (cm^2/g) appears. This condition is undoubtedly a conservative one, since some stabilization results from the implicit treatment of the radiation energy. The second condition arises from the requirement that energy flowing between adjacent zones not result in growing oscillations of energy between zones:

$$\Delta t_R \leq \min_i \frac{\left(\rho \Delta R_i\right)^2 \left(\kappa_R\right)_i \left(C_v\right)_i}{1.07 \times 10^{13} \theta_i^3} \tag{37}$$

where κ_R (cm^2/g) is the Rosseland mean opacity and ΔR is the zone thickness. This condition is the explicit stability condition for the (equilibrium) radiation diffusion equation. Again, the condition may be somewhat conservative (perhaps even superfluous), since part of the exchange takes place via the stable radiation energy equation.

1.4. HOW TO USE NON-EQUILIBRIUM DIFFUSION SUBROUTINES

This section contains information useful to the person who desires to perform calculations with the non-equilibrium diffusion subroutines in the SPUTTER code. Criteria are presented for choosing between DRADTN and ERADTN subroutines, code variables are related to variables of the derivations of Section 1.3, input quantities are discussed, and comments are made regarding how to control the problem and what difficulties may be encountered during the calculation.

1.4.1. Differences Between ERADTN and DRADTN

Radiation in equilibrium with material at temperature θ has a density of energy $E = a\theta^4$ which, under conditions of sufficiently high temperature or of low matter density, may become comparable with or greater than the material energy density. If such is the case, it is necessary to take into account this radiation energy in transit through the system in order properly to account for the energy balance of the problem. In the transport equation the radiation energy corresponds to the $1/c\ \partial I_\nu / \partial t$ term (sometimes called the retardation term) and gives rise to the time derivative terms in the non-equilibrium diffusion equation (Eq. 16).

As indicated in Section 1.3, the non-equilibrium diffusion equations have a substantially different form requiring more computation when the retardation terms are retained. Consequently, for problems in which radiation energy is neglibible, as is the case when

$$\theta(\mathrm{ev}) << 2 \times 10^3 \, [\rho(\mathrm{g/cm}^3)]^{1/3}$$

and when the light speed of propagation of radiation waves can be neglected, it was deemed desirable to solve the equations without considering the retardation terms. These equations are incorporated into a separate subroutine, ERADTN, which should be used for low-temperature problems. For problems in which the radiation energy is not small or in which it is of interest to take account of light speed with which radiation waves

propagate through vacuum, the equations including the retardation terms are solved in the DRADTN subroutine. The user must choose which of these two subroutines to incorporate into his code with the remaining desired SPUTTER subroutines. Fortunately, most of the control quantities are the same for the two codes. Exceptions are noted below, in particular the DRADTN dump tape.

1.4.2. Glossary of Code Variables

In Table I the variable quantities used in the DRADTN and ERADTN subroutines are correlated with the quantities defined in Section 1.3, where the equations are derived. In addition, a brief word description of the variable is given. Only those variables which have a use which is unique to the non-equilibrium diffusion subroutines (there are a few exceptions) are included. Consequently, a number of quantities appearing in these routines but also used in other parts of SPUTTER are not found in Table I; reference should be made to the SPUTTER report for these quantities. Most of the entries in the table are used in both routines; the few appearing only in DRADTN are distinguished by an asterisk (*).

1.4.3. Glossary of Input Quantities

Table II contains the quantities needed to control the calculations of the non-equilibrium diffusion subroutines, and information on how to establish their values. The first column contains the decimal location in common storage of the quantity, as required for card input. The second column contains the variable FORTRAN name. The third column contains a description of the quantity. Finally, the fourth column contains a typical value of the quantity. In some cases this value represents a recommended one, (e.g., AC); in other cases, merely a typical one (e.g., GA).

After having chosen between the DRADTN and ERADTN subroutines, it is necessary to make additional selections to determine the values of input quantities. Some comments regarding these selections follow.

Table I

GLOSSARY OF CODE VARIABLES

Code	Symbol	Quantity	Units
RHO(I)	E_i^{n+1}	Radiation energy density	erg/cm^3
X2(I)	$\tilde{F}_i^{n+1}$	Area-integrated flux (per volume factor)	erg/sec
ER(I)	---	Material radiative heating rate (per zone and per volume factor)	erg/sec
PDFU(I)	P_i	Coefficient of flux difference in first moment equation	cm [illegible]
RUC(I)	R_i	Coefficient of energy difference in second moment equation	$cm^{\alpha-1}/sec$
H2(I)	$1/4\lambda_i$	0.25 over diffusion mean free path (Rosseland av.)	cm^{-1}
H(I)	$c\mu_i/2$	Absorption coefficient times half light speed (Planck av.)	sec^{-1}
X6(I)	$b_j\,\theta_i^4$	Integral of Planck function over j^{th} frequency group.	$(ev)^4$
SU(I)	$c\mu_i b_j \varphi_i$	Radiation source function	$erg/cm^3 sec$
Q1(I)	θ_i^4	Fourth power of temperature	$(ev)^4$
Q37(I)	$\ln\,\theta_i$	Logarithm of temperature	---
Q38(I)	$\ln\,\tau_i$	Logarithm of specific volume	---
SUMX2(I)	$\sum_j \tilde{F}_i^{n+1}$	Sum over frequency groups of flux	erg/sec
SUMRHO(I)	$\sum_j E_i^{n+1}$	Sum over frequency groups of radiation energy	erg/sec
GU(I)	g_i	Coefficient of E_{i+1} in recurrence for E_i	---
HU(I)	h_i	Inhomogeneous term in recurrence for E_i	erg/cm^3

Table I (Continued)

Code		Symbol	Quantity	Units
OSX2(I)	*	$\sum_j \tilde{F}_i^n$	Sum over frequency groups of old flux	erg/sec
FLUX(I)		---	Value of left-hand boundary flux for GL > 0.5. Formed in the TQUE4 subroutine.	$(ev)^4$
OLDTH(I)		θ_i^n	"Old" temperature stored during iteration	ev
OLDE(I, IHNU)	*	E_i^n	"Old" radiation energy for use in DRADTN	erg/cm^3
OLDF(I, IHNU)	*	$\tilde{F}_i^n$	"Old" flux for use in DRADTN	erg/sec
WSB		---	Total internal energy; used in time interval criterion	erg
WSBB		---	Zone internal energy, used in time interval criterion	erg
THTAMX		θ_{max}	Largest of zone and boundary temperatures	ev
RDTR		$1/\Delta t_R$	Reciprocal of radiation time interval	sec^{-1}
RCDT	*	$1/4c\Delta t_R$	Reciprocal of distance light travels during time interval	cm^{-1}
TSLH		$\alpha r_1^{\alpha-1}$	Area factor for left-hand flux boundary condition	$cm^{\alpha-1}$
TSRH		$\alpha r_I^{\alpha-1}$	Area factor for right-hand flux boundary condition	$cm^{\alpha-1}$
BBSL		$b_j \theta_L^4$	Left-hand boundary Planck integral	ev^4
BBR		$b_j \theta_R^4$	Right-hand boundary Planck integral	ev^4
BETA1		β_1	Extrapolation coefficient for left-hand boundary energy	---
BETA2		β_2	Extrapolation coefficient for right-hand boundary energy	---
HNU		$h\nu_j$	Lower photon energy boundary of group j	ev

Table I (Continued)

Code	Symbol	Quantity	Units
HNUP	$h\nu_{j+1}$	Upper photon energy boundary of group j	ev
HNU4	$h\nu_j^4$	Fourth power of $h\nu_j$	ev^4
HNU4P	$h\nu_{j+1}^4$	Fourth power of $h\nu_{j+1}$	ev^4
H3M	$(\kappa\rho\Delta r)_-$	Optical depth of zone to left of interface; used in flux gradient	---
H3P	$(\kappa\rho\Delta r)_+$	Optical depth of zone to right of interface; used in flux gradient	---
BNTH	θ_i^{n+1}	Estimate of new temperature; used in iteration	ev
AU	A_i	Coefficient of E_{i-1} in radiation energy linear equation	---
BU	B_i	Coefficient of E_i in radiation energy linear equation	---
CU	C_i	Coefficient of E_{i+1} in radiation energy linear equation	---
DU	D_i	Inhomogeneous term in radiation energy linear equation	---
	*	DRADTN only	

Table II

GLOSSARY OF INPUT QUANTITIES

Common Location	Variable Name	Description	Typical Value
26	LMDA(26)	DRADTN only. Upon restart, the second data packet must contain a card setting LMDA(26) = 0.0. This causes the tape containing OLDE and OLDF to be read to obtain starting values.	0.0
44	KMAX	Frequency group indicator. Zero gives grey, nonzero, multifrequency.	0.0
75	BOILB	Maximum number of radiation subcycles permitted. Set to NTIMES in subroutine.	10.0
77	CVB	Iteration control. Zero gives single pass, nonzero, double pass with time-centered coefficients. Used to set the flag NVEZ.	0.0
78	SLUG	Time interval criterion. Maximum permissible fractional zone energy change per cycle.	0.1
79	ALPHA	Geometry selector. All values permissible for non-equilibrium diffusion: 1, slab; 2, cylinder; 3, sphere.	1.0
81	HVB	Implicit selector. When KMAX = 0.0, a nonzero value gives fully implicit equations; otherwise partially implicit equations with time step subject to stability.	1.0
87	CB	Used to minimize the number of frequency groups calculated for multi-frequency problems. Merges into one group all groups having lower frequency boundary greater than THTAMX. Too many groups merged will lead to call UNCLE unless CB is half-integral. Operative only in ERADTN.	10.0

Table II (Continued)

Common Location	Variable Name	Description	Typical Value
88	GA	Left boundary condition indicator. Operative only if no pusher. (Pusher present prescribes blackbody flux.) GA < 0 gives zero net flux; GA = 0 gives vacuum to the left; GA > 0 gives UNCLE call.	0.0
90	GL	Right boundary condition indicator. GL < 0 gives zero net flux; GL = 0 gives vacuum to the right; GL = 0.5 gives blackbody flux specified by THETA(IM+1); GL > 0.5 gives flux specified via FLUX(I) in the TQUE4 subroutine.	0.5
126	AC	Criterion in diffusion mean free path (H2(I)) calculation. If optical depth is greatly different in adjacent zones, the optically thinner zone is used instead of forming an average.	0.3
147	EDITMF	Same as S12. Nonzero value gives multifrequency print which also serves as a debug print.	0.0
152	S17	Old implicit switch which sets S9. Note changed from previous usage.	---
8466	TELM(25)	Multiplied to change radiation time interval after all criteria have been applied.	1.0
8478	TELM(37)	Fraction of internal energy of the entire mesh which each zone must exceed before energy change of that zone is tested (see SLUG) in the time interval calculation.	0.003
8858	SOLID(10)	Switch to permit Rosseland mean to be substituted for Planck mean if value is not zero.	0.0

The frequency treatment decided on is very important for the speed and accuracy of the calculation. Two situations permit a monofrequency, or grey, calculation. If the medium is optically thick it is usually permissible to perform a grey calculation. However, it is necessary that the medium be thick to all relevant frequencies, i. e., those which transport appreciable energy. Exceptions occur when sharp temperature changes exist in the medium, such as at radiation or shock fronts and at boundaries. If they are transient or localized, it is usually permissible to perform the grey calculation. At the other extreme, if the medium is optically thin in all important parts of the spectrum, the grey calculation can be performed. In both of these situations it is sometimes desirable to find the spectrum of the radiation in or, more commonly, emerging from the material. It is not necessary to run the calculation with frequency groups through the entire problem history in this case. Instead, the grey calculation can be edited with a "snapshot" multifrequency calculation at desired times. When the material is intermediate between these situations, the multifrequency calculation is necessary. However, it is under these conditions of intermediate optical thickness that the non-equilibrium diffusion approximation is least reliable.

The grey calculation with KMAX = 0. 0 permits the implicit indicator HVB to be set to a nonzero value, thereby releasing the time interval from the control of stability criteria and leaving it subject only to accuracy considerations. The implicit option should be exercised when possible (the option exists only to permit test investigations of the code). When a multifrequency calculation is required, the partially implicit solution is mandatory. Consequently, multifrequency calculations are lengthy not only because the calculation is repeated for each frequency group, but because the time interval may be reduced substantially below the value for implicit calculation. When there is doubt about the necessity for groups, one can first calculate a grey solution and then compare the resulting radiation fluxes with those obtained with a few "snapshot" multifrequency

calculations. Substantial differences indicate that the multifrequency calculation is required ab initio. Frequently, the grey calculation is not wasted, since the information about zoning of the problem can be incorporated into the subsequent calculation.

No good criterion for the decision about iteration exists. In general, iteration almost doubles the computing time. Iteration may be warranted if the increased accuracy of the solution permits a time interval which is more than twice as large as that used in the solution without iteration. Whether the accuracy is substantially affected depends on both the variability of the coefficients of the radiation equations (which is different for the implicit and partially implicit forms of the equations) and the rapidity of change of the solution with time. When iteration is performed, the accuracy criterion (SLUG) should be relaxed.

The optical depth between zone centers required in the gradient term of the radiation flux is difficult to evaluate accurately in regions where the mean free path changes rapidly in space, as near the front of a radiation wave. No completely satisfactory prescription is yet available, but a method containing the variable AC is available in the subroutines. This quantity, which controls the transition from using an average of optical depths of neighboring zones when the optical depths do not differ greatly to using the smaller optical depth when the difference is large, has been found to give accurate results for a diffusion test problem when AC = 0.3. Further improvement would result from a prescription incorporating the effect of temperature gradient on mean free path within a zone.

Boundary conditions at the two faces of the shell of material being calculated are determined from several options. When the spherical or cylindrical shell is not hollow, the boundary condition at the origin is irrelevant, but GA $\leq$ 0 should be set. When no pusher exists, the left boundary can be made to give zero net flux to simulate a perfectly reflective region on the left or to permit radiation to flow unimpeded from the material to simulate a vacuum on the left. Similar options are available

for the right boundary with the addition of a blackbody boundary condition and a boundary flux. The blackbody condition simulates the effect of a hohlraum at temperature THETA(IM+1) shining on the right boundary. The boundary flux condition is a special-purpose feature, making use of the TQUE4 routine. With it the frequency dependent flux found in a fireball can be applied to the right surface of the material. Quite small modifications of the subroutines could make these last two options applicable also to the left boundary. An alternative method of applying an external radiation boundary condition is through a source routine which forms an energy source in the material as determined by the rate of energy absorption at various depths. An example is the QUE4 subroutine for incident X-rays.

The time interval of the calculation is determined by both accuracy and stability criteria. The calculation of radiation flow can be performed at a smaller time interval than the hydrodynamics, so that a number of subcycles of the radiation limited by BOILB are calculated every cycle. It is not desirable to allow the number of subcycles to become very large. First, the calculation time for other parts of the cycle is not large compared with the radiation, so no appreciable saving results. Second, substantial radiation flow during subcycles may induce other changes which, when finally calculated on the next cycle, may be catastrophically large. Third, a large amount of computation time is spent during which no information is available about the progress of the problem. Consequently, it is desirable to limit the time interval, if necessary, by control cards so that a limited amount of subcycling occurs. When a strong external source is applied to the surface of the material, transients are established which require an unusually small time interval for a few cycles. Control card reduction of the time interval is usually necessary during the first few cycles.

1.4.4. Subroutines Called by DRADTN and ERADTN

Within the subroutine codes it is assumed that two special-function subroutines and dependent subroutines which are an integral part of the radiation calculation are available. These subroutines are described below.

PLNKUT (α_1, α_2). This function returns the partial Planck function defined by

$$\frac{15}{\pi^4} \int_{\alpha_1}^{\alpha_2} \frac{u^3 du}{e^u - 1}$$

It is a function of two variables, $\alpha_1 = h\nu_1/\theta$ and $\alpha_2 = h\nu_2/\theta$ ($\alpha_1 < \alpha_2$). The routine is described in Ref. 9.

KAPPA (i_1, i_2). This routine returns values of the Rosseland opacity κ_R and the Planck opacity κ_P for the temperatures, densities, and materials appropriate to the zones having indices from i_1 to i_2. For problems specifying more than one frequency group, the appropriate frequency group average coefficients are provided as well as the quantities averaged over the entire spectrum.

In addition, use is made of the subroutines UNCLE, DVCHK, and NONEQ.

Boundary flux values are formed in a special TQUE4 subroutine and used when GL > 0.5 via the FLUX(I) array. These values are the result of integrating the frequency group intensities to obtain the radiation current incident on the boundary. The TQUE subroutine processes the AFWL "users tape" to obtain radiation intensities resulting from fireball calculations.

1.5. TEST PROBLEMS

Test calculations have been performed to evaluate the accuracy of the non-equilibrium diffusion method. These calculations are of two

classes. Idealized problems (slab penetration, isothermal sphere cooling) have been compared with corresponding transport solutions. "Real" problems dealing with interaction, slab penetration, and fireball growth have been computed. On the basis of the results, modifications of mean free path averaging and boundary condition formulation have been made.

Solutions for comparison have been calculated with subroutines, for radiation transport from the SPUTTER code (Ref. 5). These routines are applicable only to spherical geometry (SRADTN) and slab geometry (PRADTN), so the comparison calculations have been restricted to these two geometries.

All of the idealized calculations are without hydrodynamics and use a gray and temperature independent absorption coefficient.

The first calculation applies to a semi-infinite absorbing medium initially cold. At $t = 0$ an isotropic source shines on the surface of the medium and progressively heats it. The initial heating phase is followed by a transition to a diffusive solution in which a wave penetrates progressively more slowly into the interior of the slab. Numerical calculations of this problem have also been made by Barfield (Ref. 10). Both the DRADTN and ERADTN equations have been tested on the problem in which there are four zones per mean free path in the medium. In Fig. 1 the fluxes entering the medium versus time are compared for the two. The only appreciable difference occurs at early time. In Fig. 2, plots of temperature profiles for the ERADTN and PRADTN calculations are compared. Largest deviations appear at early time and near the wave front. Results obtained with DRADTN for this problem are substantially the same as those obtained with ERADTN.

The second idealized problem describes the cooling of a sphere of gas in vacuum. Initially, the sphere is isothermal and contains a fixed number of absorption mean free paths in the radius. Calculations have been performed for three thicknesses of sphere: 1, 2, and 5 mean free paths per radius, in each of which 20 radial zones are used. Comparisons

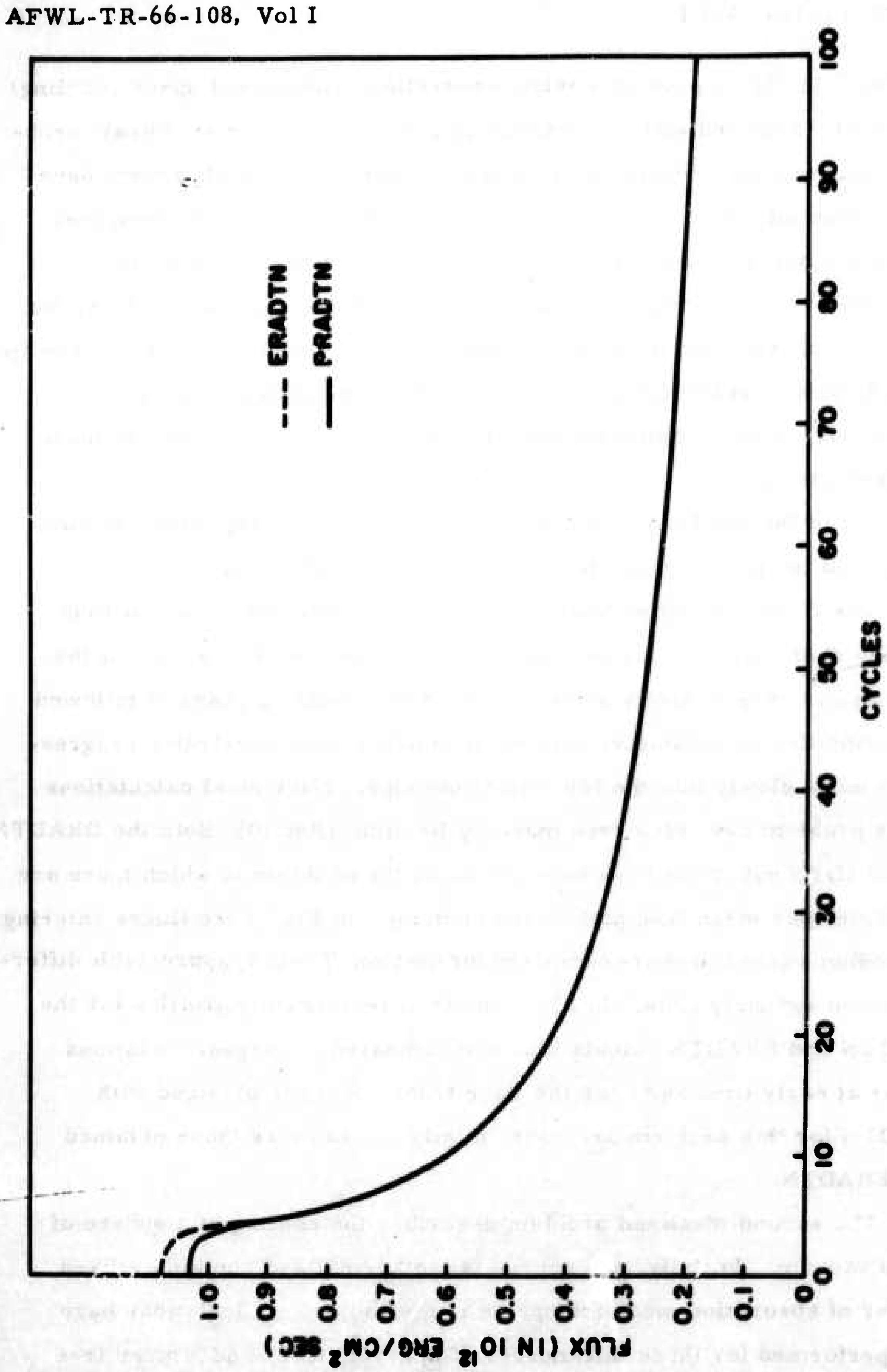

Figure 1. Slab Penetration Fluxes

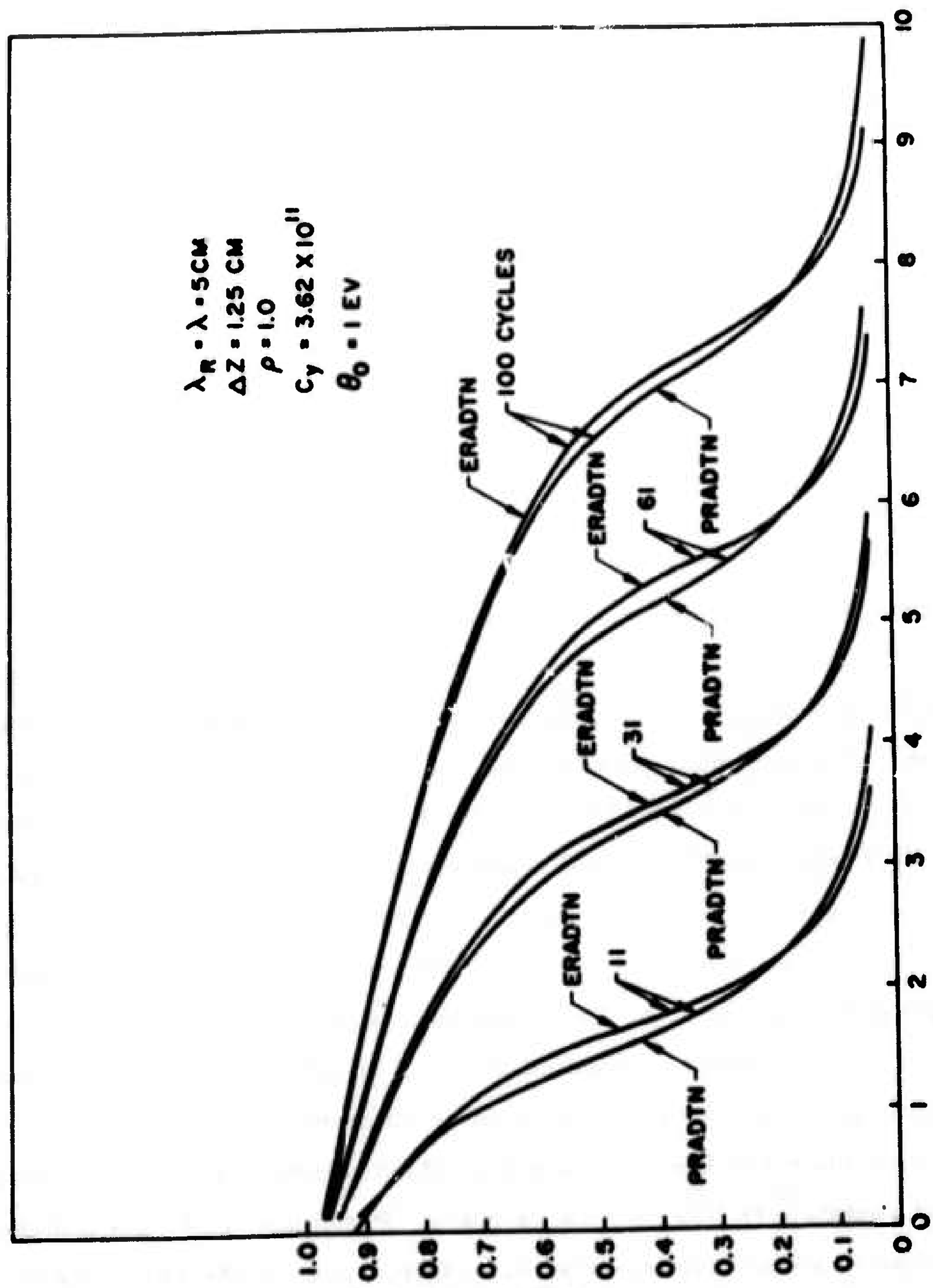

Figure 2. Slab Penetration Temperature Profiles

of ERADTN with SRADTN for these cases are shown in Fig. 3, where the temperature is plotted as a function of time for the 2 mean free path case. In Figs. 4 and 5, the corresponding curves for the 1 and 5 mean free path cases are given. Temperature differences of several percent are found. It is to be expected that both optically thick and optically thin cases will be more accurate. In Fig. 6 the flux at the surface of the sphere is shown as a function of time. The comparison calculations are sufficiently close (never differing by more than 2%) so as to be represented by a single curve for each case. In the one case in which DRADTN was calculated, similar results were obtained but oscillation was observed.

As indicated by the above example, DRADTN presently gives less satisfactory results due to bounded oscillations having small damping. This problem has been improved by recentering in time of the exchange term as indicated in Section 1.3.

Additional test problems corresponding to situations arising in applications of SPUTTER have been run. The ERADTN and PRADTN equations have been compared, and agree well for the problem of radiation impinging on an opaque slab and inducing radiation penetration preceded by a strong shock wave. A cycle of the BLUE GILL fireball problem has been repeated with ERADTN and SRADTN. While results are quite similar in the fireball interior, the fluxes are quite different in the free streaming region outside. The latter appear to point to the failure of the radiation energy to diverge in the Eddington approximation when radiation is emitted from a compact source. This very recently identified problem is still under consideration; incorporating parts of the second moment equation may help solve it. An interaction problem has been compared in which ablation of a target induced by thermal radiation falling on it takes place. Preliminary results indicate agreement after a short transient period. Differences in the early result may be reduced by a modified boundary condition not yet tested for this problem.

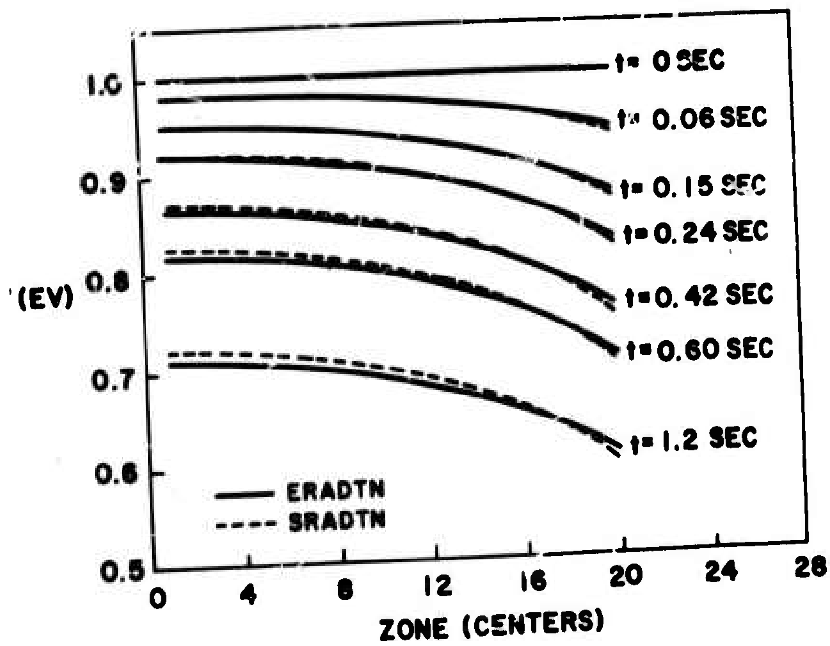

Figure 3. Spherical Emission Test Problem, $\Delta t = 0.03$, $\kappa_R = \kappa_P = 0.2$

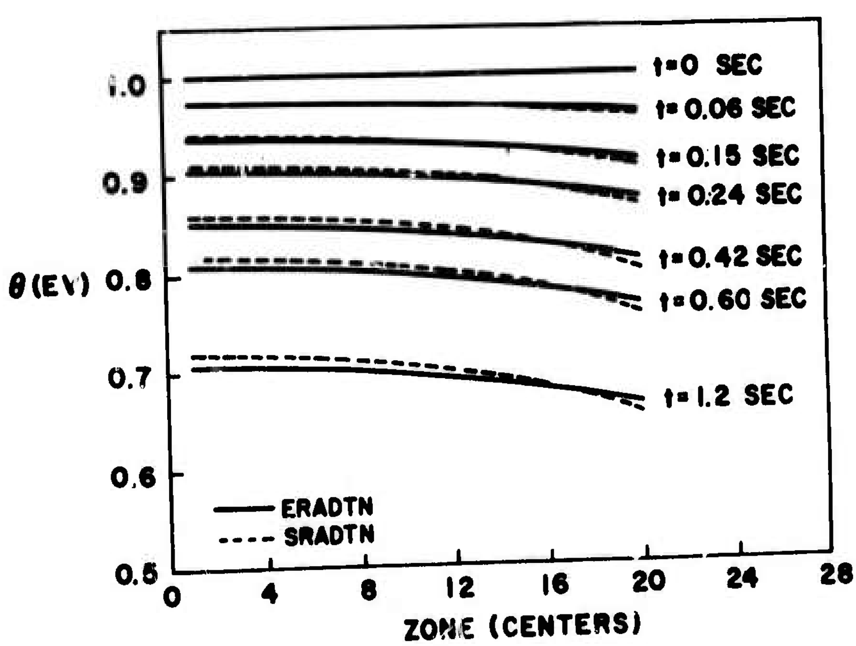

Figure 4. Spherical Emission Test Problem, $\Delta t = 0.03$, $\kappa_R = \kappa_P = 0.1$

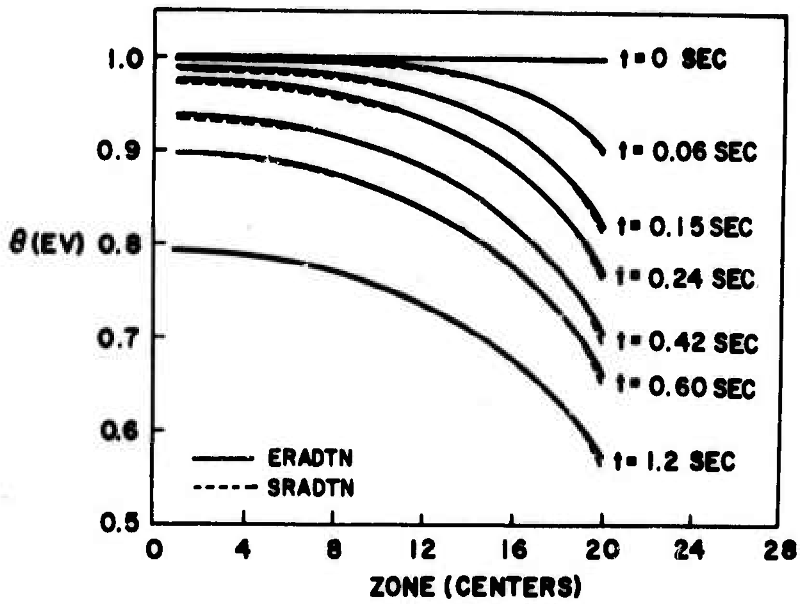

Figure 5. Spherical Emission Test Problem, $\Delta t = 0.03$, $\kappa_R = \kappa_P = 0.5$

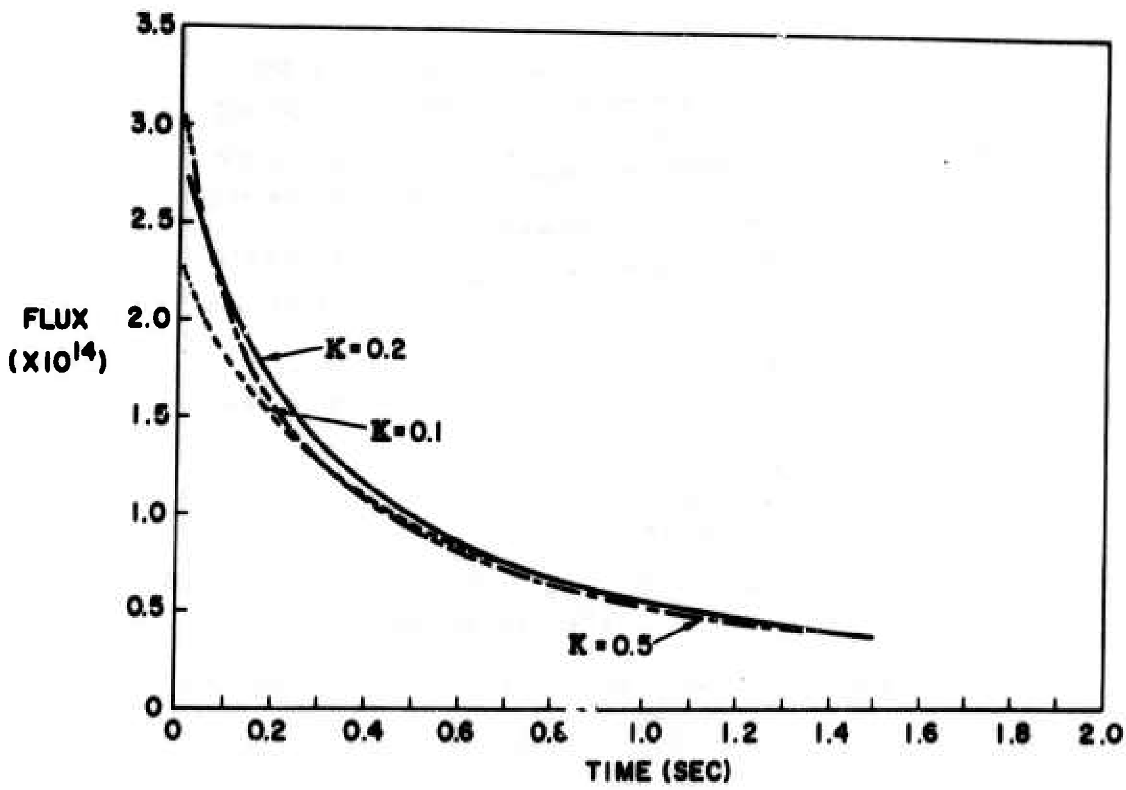

Figure 6. Flux Versus Time for Spherical Emission Test Problem, t = 0. 03

The findings to date show very satisfactory agreement for slab problems and indicate that there are many potential applications of the non-equilibrium diffusion equations. How generally applicable the method can be made is not yet known.

1.6. APPENDIX: STABILITY ANALYSIS

The stability analysis of the difference equations for non-equilibrium diffusion is partially developed in this section. The defining equations for this physical process are given.

The stability theory of finite difference equations is sufficiently stated in a book by Richtmyer (Ref. 11). He gives the following definition of stability:

Definition

If a finite difference scheme is given by

$$u^{n+1} = c(\Delta t)u^n$$

where u^n is an m-column vector and $c(\Delta t)$ is an mxm array, the system is said to be stable if there exists a τ such that the sequence $\left\{ \|c(\Delta t)\|^j \right\}_{j=0}^{n}$ is uniformly bounded, where $0 < \Delta t < \tau$.

Consistent with this definition, a sufficient condition for stability is that the spectral radius of $c(\Delta t)$ be less than 1. This theorem is developed and proved by Richtmyer (Ref. 11).

The difference equations proposed for defining non-equilibrium diffusion are

$$(1)\ \frac{E^{n+1} - E^n}{\Delta t^n} + \frac{P_i}{2}(F^{n+1}_{i+1} - F^{n+1}_i + F^n_{i+1} - F^n_i) = \frac{c\mu_i}{2}(2b_j\phi_i - E^{n+1}_i - E^n_i)$$

$$(2)\ \frac{F^{n+1}_i - F^n_i}{c\Delta t^n} + 2R_i(E^{n+1}_i - E^{n+1}_{i-1} + E^n_i - E^n_{i-1}) = \frac{-1}{2\lambda_i}(F^{n+1}_i + F^n_i)$$

$$(3)\ \phi_i^{n+1} = \phi_i^n + f_i\left[q_i - \left(P_i + \frac{\partial E_m}{\partial \tau}\right)\frac{\partial \tau}{\partial t} - \frac{c}{2\rho}\sum_j \mu_i\,(2b_j\phi_i - E_i^{n+1} - E_i^n)\right]$$

where the terms are defined as in Section 1.3. The first two equations are the defining relations for the pertinent moments of the intensity. The third equation expresses the conservation of energy.

As the difference equations are now stated, a stability condition cannot be found as a function of the parameters. Various assumptions are employed to reduce the system to one amenable to solution. These assumptions are summarized as follows:

1. Ignore hydrodynamics
2. No energy sources, i.e., $q_i = 0$
3. Monofrequency
4. Plane geometry
5. Scattering is negligible

With these assumptions the system of equations becomes

$$(1)\ \frac{E_i^{n+1} - E_i^n}{\Delta t} + \frac{1}{2\Delta x}(F_{i+1}^{n+1} - F_i^{n+1} + F_{i+1}^n - F_i^n) = \frac{c\mu}{2}(2\phi_i - E_i^{n+1} - E_i^n)$$

$$(2)\ \frac{F_i^{n+1} - F_i^n}{c\Delta t} + \frac{c}{6\Delta x}(E_i^{n+1} - E_{i-1}^{n+1} + E_i^n - E_{i-1}^n) = -\frac{\mu}{2}(F_i^{n+1} + F_i^n)$$

$$(3)\ \phi_i^{n+1} = \phi_i^n - \left(\frac{4a\,\theta_i^3}{(C_v)_i}\right)\frac{c\Delta t\mu}{2\rho}(2\phi_i - E_i^{n+1} - E_i^n)$$

With this system of equations two possible special cases may be investigated. Consider first that the material energy is much larger than the radiation energy. This requirement is equivalent to $\phi \approx$ constant for some time interval τ. In this time interval one can investigate the stability of partially implicit equations (1) and (2) above. Expanding E and F into Fourier components, one finds, after some reduction, that the amplification matrix $C(\Delta t)$ is given by

$$C(\Delta t) = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}$$

where

$$C_{11} = \frac{\left(1 + \frac{c\mu\Delta t}{2}\right)\left(1 - \frac{c\mu\Delta t}{2}\right) - \frac{c^2}{3}\left(\frac{\Delta t}{\Delta x}\right)^2 \sin^2 k \frac{\Delta x}{2}}{M}$$

$$C_{12} = -\frac{2\frac{\Delta t}{\Delta x}\, i \sin k \frac{\Delta x}{2}\, e^{i(k\Delta x/2)}}{M}$$

$$C_{21} = -\frac{\frac{2c^2}{3}\frac{\Delta t}{\Delta x}\, i \sin k \frac{\Delta x}{2}\, e^{-i(k\Delta x/2)}}{M}$$

$$C_{22} = \frac{\left(1 - \frac{c\mu\Delta t}{2}\right)\left(1 + \frac{c\mu\Delta t}{2}\right) - \frac{c^2}{3}\left(\frac{\Delta t}{\Delta x}\right)^2 \sin^2 k \frac{\Delta x}{2}}{M}$$

$$\begin{pmatrix} E^{n+1} \\ F^{n+1} \end{pmatrix} = C(\Delta t)\begin{pmatrix} E^{n} \\ F^{n} \end{pmatrix}$$

$$M = \left(1 + \frac{c\mu\Delta t}{2}\right)^2 + \frac{c^2}{3}\left(\frac{\Delta t}{\Delta x}\right)^2 \sin^2 k\frac{\Delta x}{2}$$

A sufficient condition for stability is that the eigenvalues of $C(\Delta t)$ lie within the unit circle. The eigenvalues are given by

$$\lambda^2 - T\lambda + \Delta = 0 \qquad \text{where } T = \text{trace}\,(C(\Delta t))$$
$$\Delta = \det\,(C(\Delta t))$$

The conditions that the roots lie within the unit circle can be found from the Routh criterion (Ref. 12) after making the transformation $\lambda = (\omega + 1)/(\omega - 1)$. This

transformation maps the interior of the unit circle into the left half complex plane. Making the substitution, one has

$$\omega^2(1 + \Delta - T) + 2\omega(1 - \Delta) + 1 + T + \Delta = 0$$

For a second order equation the Routh criterion requires that the coefficients of the equation be positive if the roots of the equation are contained within the left half plane. Thus, the conditions are given by

$$(1)\ \Delta < 1$$
$$(2)\ |T| < \Delta + 1$$

After some algebraic manipulation, one can show that conditions (1) and (2) are always satisfied independent of Δt. Thus, the system is unconditionally stable.

The second case in which the stability can be analyzed is the situation in which spatial homogeneity exists. The difference equations can then be written as

$$(1)\ E^{n+1} - E^n = g[\alpha\phi^n + (1-\alpha)\phi^{n+1} - \beta E^{n+1} - (1-\beta)E^n]$$

$$(2)\ F^{n+1} - F^n = -g(\gamma F^{n+1} + (1-\gamma)F^n)$$

$$(3)\ \phi^{n+1} - \phi^n = -\lambda g[\alpha\phi^n + (1-\alpha)\phi^{n+1} - \beta E^{n+1} - (1-\beta)E^n]$$

where $g = c\mu\Delta t$, $\lambda = 4a\theta^3/\rho C_v$, and $0 \leq \alpha \leq 1$, $0 \leq \beta \leq 1$, and $0 \leq \gamma \leq 1$. One notes that the second equation is always stable if $\gamma \geq 1/2$. For the coupled system of Eqs. (1) and (3), one has the following system:

$$\begin{pmatrix} E^{n+1} \\ \phi^{n+1} \end{pmatrix} = C(\Delta t)\begin{pmatrix} E^n \\ \phi^n \end{pmatrix}$$

where $C(\Delta t)$ is as defined previously.

The elements of the amplification matrix are found to be

$$C_{11} = [[1 - g(1 - \beta)] [1 + \lambda g(1 - \alpha)] + \lambda g^2 (1 - \alpha)(1 - \beta)] / Q$$

$$C_{21} = [\beta\lambda g[1 - g(1 - \beta)] + [1 + g\beta] [\lambda g(1 - \beta)]] / Q$$

$$C_{12} = [g\alpha[1 + \lambda g(1 - \alpha)] + g(1 - \alpha)(1 - \lambda g\alpha)] / Q$$

$$C_{22} = [\beta\lambda g^2 \alpha + (1 + g\beta)(1 - \lambda g\alpha)] / Q$$

where $Q = (1 + g\beta) [1 + \lambda g(1 - \alpha)] - \beta\lambda g^2(1 - \alpha)$.

After some reduction, one finds

$$T = \frac{2 - g(1 - 2\beta) + \lambda g(1 - 2\alpha)}{1 + g\beta + g\lambda(1 - \alpha)}$$

and

$$\Delta = \frac{1 - g(1 - \beta + \lambda\alpha)}{1 + g\beta + \lambda g(1 - \alpha)}$$

It is interesting to note that $T = \Delta + 1$. Thus, the characteristic roots are given by

$$\lambda^2 - (\Delta + 1)\lambda + \Delta = 0$$

or

$$\lambda_{1,2} = \frac{\Delta + 1 \pm \sqrt{(\Delta + 1)^2 - 4\Delta}}{2}$$

$$= \begin{cases} \Delta \\ 1 \end{cases}$$

Therefore, for all parameter variations the roots are real and distinct.

The coefficients α, β determine whether the system of equations is implicit and unconditionally stable. For various parameter variations the stability conditions are listed in Table III. It is clear from Table III that the system of equations is unconditionally stable when the equations are partially or fully implicit in both E and ϕ.

Table III

STABILITY CONDITIONS AND ORDER OF ACCURACY

Case	α	β	Description	Accuracy	Stability Conditions
1	0	1	Fully implicit	1st order	Uncond. stab.
2	1/2	1	Fully imp. in E; partially imp. in ϕ	1st order	Uncond. stab.
3	0	0	Explicit in E; fully imp. in ϕ	1st order	$\Delta t < \dfrac{2}{c\mu\left(1 - \dfrac{4a\theta^3}{\rho C_v}\right)}$
4	1	1/2	Part. imp. in E; exp. in ϕ	1st order	$\Delta t < \dfrac{2\rho C_v}{4c\mu a\theta^3}$
5	1	0	Explicit	1st order	$\Delta t < \dfrac{2}{c\mu\left(1 + \dfrac{4a\theta^3}{\rho C_v}\right)}$
6	0	1/2	Part. imp. in E; fully imp. in ϕ	1st order	Uncond. stab.
7	1/2	1/2	Part. imp. in both E, ϕ	2nd order	Uncond. stab.

For this simplified system of equations another problem of interest is the amount of damping in the system. For the second equation one notes that

$$F^{n+1} = \left(\frac{1 - g(1 - \gamma)}{1 + g\gamma}\right) F^n$$

or

$$F^{n+1} = \left[\frac{1 - g(1 - \gamma)}{1 + g\gamma}\right]^n F^o$$

Thus, the solution for the flux has a damping coefficient given by $[1 - g(1 - \gamma)]/(1 + g\gamma)$ when $\gamma \geq 1/2$.

From matrix theory (Ref. 13) one knows that there exists a similarity transformation P such that

$$P^{-1} C P = \begin{bmatrix} 1 & 0 \\ 0 & \Delta \end{bmatrix}$$

or

$$C = P \begin{bmatrix} 1 & 0 \\ 0 & \Delta \end{bmatrix} P^{-1}$$

Thus, the equations can be rewritten as

$$\begin{pmatrix} E^{n+1} \\ \phi^{n+1} \end{pmatrix} = (P) \begin{pmatrix} 1 & 0 \\ 0 & \Delta \end{pmatrix} (P^{-1}) \begin{pmatrix} E^n \\ \phi^n \end{pmatrix} .$$

By successive subsitution, one has

$$\begin{pmatrix} E^{n+1} \\ \phi^{n+1} \end{pmatrix} = P \begin{pmatrix} 1 & 0 \\ 0 & \Delta^n \end{pmatrix} P^{-1} \begin{pmatrix} E^o \\ \phi^o \end{pmatrix}$$

At this point the significance of the roots 1 and Δ becomes apparent. The root 1 corresponds to the steady state solution, and the root Δ is the transient part of the solution. Hence, the damping in the system can be controlled by varying Δ.

1.7. APPENDIX: LISTING OF ERADTN AND PRADTN

```
      SUBROUTINE  RADTN
C*******************************************************************
C*                    S P U T T E R   C O M M O N                  **
C                                                                  *
      COMMON   LMDA(37), NR     , NSMLR , IA     , IB     , ICA    , ICB    ,
     1    KMAX   , BLANK1, BLANK2, BLANK3, IAP1   , IBP1   , ICAP1  , ICBP1  ,
     2    II     , IG     , NRAD   , BLANK4, IAM1   , IBM1   , ICAM1  , ICBM1  ,
     3    IIP1   , IGM1   , IALPHA, BLANK5, TH     , TMAX   , BLANK6, DELPRT,
     4    FREQ   , CNTMAX, AR     , ASMLR , PUSHA  , PUSHB  , BOILA  , BOILB  ,
     5    CVA    , CVB    , SLUG   , ALPHA  , HVA    , HVB    , HCA    , HCB    ,
     6    EMINA  , EMINB  , CA     , CB     , GA     , GB     , GL     , GR     ,
     7    RHOL   , RHOR   , EPIO   , EPSI   , RIA    , RIB    , RDIA   , RDIB   ,
     8    RPIA   , RPIB   , RPDIA  , RPDIB  , TPRINT, TA     , TB     , TC
      COMMON      TD     , TE     , DTH2   , DTH2P  , DTH1   , DTRMIN, DTMAX  ,
     1    DTMAX1, DTMAX2, DTMAX3, DTR    , SWITCH, CO     , CMIN   , DELTA  ,
     2    GAMA   , WCRIT  , SIGMAQ, AC     , ACO3T4, CNVRT  , SUMRA  , SUMRB  ,
     3    ROIA   , ROIAM1, ROIB   , ROIBP1, GMS    , S1     , S2     , S3     ,
     4    S4     , S5     , S6     , S7     , S8     , S9     , S10    , S11    ,
     5    S12    , S13    , S14    , S15    , S16    , S17    , S18    , S19    ,
     6    S20    , EO     , FO     , TAU    , ZERO   , R     (152), DELTAR(152),
     7  ASQ    (152), RD     (152), VD     (152), RDD    (152), SMLR   (152),
     8  DELR   ( 37), P      (152), P1     (152), PB     (152), PB1    (152)
      COMMON          P2     (152), SV     (152), RHO    (152), THETA  (152),
     1  W      (152), E      (152), EI     (152), EK     (152), A      (152),
     2  V      (152), G      (152), D      (152), C      (152), X2     (152),
     3  X3     (152), X4     (152), X5     (152), X6     (152), X7     (152),
     4  SMLA   (152), SMLB   (152), SMLC   (152), SMLD   (152), SMLE   (152),
     5  EC     (152), ER     (152), SMLQ   (152), SMLH   (152), BIGA   (152),
     6  BIGB   (152), CV     (152), BC     (152), BR     (152), CHIC   (152),
     7  CHIR   (152), CAPAC  (152), CAPAR  (152), CRTC   (152), CRTR   (152),
     8  CRTPC  (152), GOFR   (152), FEW    (152), CAR    (152), OKLM   ( 37)
      COMMON          TELM   ( 37), EKLM   ( 37), ELM    ( 37), FCLM   ( 37),
     1  FRLM   ( 37), WLM    ( 37), QLM    ( 37), AMASNO( 37), CHRNO  ( 37),
     2  ZP1    ( 37), ZP2    ( 37), SOLID  ( 37), ECHCK  ( 37), RK     (104),
     3  RL     ( 37), RHOK   (104), RDK    (104), THETAK(104), TEMP   ( 16),
     4  HEAD   ( 12), MAXL          , MAXLM
C*                                                                 **
C*******************************************************************
C
      DIMENSION  RUC(1), OSX2(1), H2(1), Q1(1), GU(1), SU(1), HU(1)
      DIMENSION  PDFU(1), SUMRHO(1), H(1), SUMX2(1), OLDTH(1)
      DIMENSION  Q37(1), Q38(1)
      DIMENSION OLDE(152,3), OLDF(152,3)
      COMMON /LINDLY/ HNU,SGNL,IHNU,NHNU,HNUP,NT,IM,IN,DHNU,THICK,NY
      COMMON/TQ/QINT1(300),QINT2(300),TITLE(12),FLUX(30)
      COMMON /CNTRL/ SCYCLE, JMULT
C
      EQUIVALENCE  (SMLA,PDFU), (SMLD,SUMRHO)
      EQUIVALENCE  (BC,OSX2),(BIGB,H),(CRTR,SUMX2),(CHIC,SU)
      EQUIVALENCE  (SMLH,GU),(CAR,Q37),(CHIR,Q38),(SMLC,OLDTH)
      EQUIVALENCE  (ACO3T4,TRDBG),(S12,EDITMF)
      EQUIVALENCE  (EC,Q1),(X7,H2),(BIGA,HU    ),(GOFR,RUC)
C
      DATA ILMDA /0/
C*******************************************************************
C                                                                  *
C                         EDITMF  SAME AS     S12                  *
C                         H       SAME AS    BIGB                  *
C                         H2      SAME AS      X7                  *
C                         OLDTH   SAME AS    SMLC                  *
C                         PDFU    SAME AS    SMLA                  *
C                         Q1      SAME AS      EC                  *
C                         RUC     SAME AS    GOFR                  *
C                         Q37     SAME AS     CAR                  *
C                         Q38     SAME AS    CHIR                  *
C                         SUMX2   SAME AS    CRTR                  *
```

```
C                         SU      SAME AS   CHIC                          *DRAD0670
C                         HU      SAME AS   HIGA                          *DRAD0680
C                         TRDBG   SAME AS AC03T4                          *DRAD0690
C                         GU      SAME AS   SMLH                          *DRAD0700
C                         SUMRHO  SAME AS   SMLD                          *DRAD0710
C                                                                         *DRAD0720
C************************************************************************DRAD0730
C                                                                          DRAD0780
C     NONEQUILIBRIUM RADIATION DIFFUSION AS IN LA-3377
C
C     FOR DRADTN AND ERADTN. NY (IN LINDLEY COMMON) IS TEMPERATURE
C     ITERATION INDEX.  THIS IS USED IN A SPECIAL DIANA THAT GOES WITH
C     DRADTN AND ERADTN.
C                                                                          DRAD0820
C************************************************************************DRAD0830
C
C          INITIALIZATION AND CALCULATION FOR NO VAPOR ZONES
C
C************************************************************************
C                                                                          DRAD0840
      CALL DVCHK(KDMY)
      NTIMES=BOILB                                                         DRAD0850
      IM=IBM1                                                              DRAD0860
      IN=IA                                                                DRAD0870
      IDMHNU = 3
      IF (KMAX .EQ. 0)  DHNU = 1.                                          DRAD0880
      IF(ZP1(26).EQ.0.) GO TO 15
C                                                                          DRAD0900
C               SAVE STUFF FROM EIONX FOR NONEQ AND RESET IN OR IM         DRAD0910
C                                                                          DRAD0920
      IF (PUSHA .LT. 0.0)   GO TO 100                                      DRAD0930
      IM = NR - 1                                                          DRAD0940
      CALL NONEQ(IM+1,4)                                                   DRAD0950
      GO TO 15                                                             DRAD0960
  100 IN = NR                                                              DRAD0970
      CALL NONEQ(IN-1,4)                                                   DRAD0980
   15 CONTINUE                                                             DRAD0990
      IMP1=IM+1                                                            DRAD1000
      INM1=IN-1                                                            DRAD1010
      INP1 = IN + 1                                                        DRAD1020
      IF (IMP1 - IN)  20, 20, 25
C                                                                          DRAD1040
C          CALCULATE BLACKBODY EMISSION AND EXIT IF NO VAPOR ZONES         DRAD1050
C                                                                          DRAD1060
   20 X2(IMP1) = 1.0275E12 * A(IMP1) * (THETA(IM)**4 - THETA(IMP1)**4)
      ER(IM)=-X2(IMP1)                                                     DRAD1080
      GO TO 1300                                                           DRAD1090
   25 NVEZ = 1
      NY = NVEZ                                                            DRAD1110
      IF(CVB.EQ.0.0) NVEZ = 2                                              DRAD1120
      VEZ = NVEZ                                                           DRAD1130
C                                                                          DRAD1150
C          FORM INTERPOLATION QUANTITIES FOR OPACITY SUBROUTINE
C                                                                          DRAD1170
      DO 1076 I=IN,IM                                                      DRAD1210
      OSX2(I) = 0.
      Q37(I)=ALOG(THETA(I))                                                DRAD1220
 1076 Q38(I)=ALOG(SV(I))                                                   DRAD1230
      OSX2(IMP1) = 0.
C
C       OBTAIN ROSSELAND AND PLANCK OPACITIES FOR ENTIRE SPECTRUM
C       (REQUIRES DIANE TAPE HAVING MONOFREQUENCY OPACITIES FIRST)
C
      IHNU = 0                                                             DRAD1240
      CALL KAPPA(IN,IM)                                                    DRAD1250
```

```
C***********************************************************************DRAD1260
C                                                                       DRAD1270
C        M I N I M U M   T I M E   S T E P   C A L C U L A T I O N      DRAD1280
C                                                                       DRAD1290
C***********************************************************************DRAD1300
      WSB = 0.0
      DO  1075  I = 1, MAXLM
 1075 WSB = WSB + ELM(I)
      DTR1=1.E10                                                        DRAD1310
      DTR2=1.E10                                                        DRAD1320
 1080 DO 1230 I=IN,IM                                                   DRAD1330
C                                                                       DRAD1340
C             CALL UNCLE IF EITHER KAPPA IS ZERO OR NEGATIVE            DRAD1350
C                                                                       DRAD1360
      IF (AMIN1(CAPAC(I), CAPAR(I)) .GT. 0.0)  GO TO 1120               DRAD1370
      S1=13.1090                                                        DRAD1380
      CALL UNCLE                                                        DRAD1390
C
C             SOLID(10) NOT ZERO GIVES ALL ROSSELAND OPTION
C
 1120 IF(SOLID(10).EQ.0.0) GO TO 1123
      TEMP(1) = CAPAR(I)
      TEMP(3) = CAPAR(I)
      GO TO 1125
 1123 TEMP(1)=SQRT(CAPAR(I)*CAPAC(I))
      TEMP(3) = CAPAC(I)
 1125 IF(0.001 - THETA(I)) 1160,1230,1230                               DRAD1480
 1160 H(I) = 0.5 * TEMP(1) / SV(I) * DELTAR(I)                          DRAD1490
      TEMP(1) = 1.E10                                                   DRAD1500
      TEMP(2) = 1.E10                                                   DRAD1510
      IF (TELM(37) .EQ. 0.0 .OR. ER(I) .EQ. 0.0)  GO TO 1170
      WSBB = E(I) * G(I)                                                DRAD1530
      IF (WSBB - TELM(37) * WSB)  1170, 1165, 1165                      DRAD1550
C                                                                       DRAD1560
C      ACCURACY CRITERION - DONE FOR FULLY AND PARTIALLY IMPLICIT CASES
C                                                                       DRAD1580
 1165 TEMP(1) = SLUG * WSBB / ABS(ER(I))
 1170 IF (KMAX .EQ. 0   .AND. HVB .NE. 0.0)  GO TO 1172                 DRAD1600
C                                                                       DRAD1610
C          STABILITY CRITERION -- BYPASSED IN FULLY IMPLICIT CASE       DRAD1620
C                                                                       DRAD1630
      TEMP(2) = CV(I) / (2.066E12*TEMP(3)*THETA(I)**3)
      TEMP(3) = TEMP(2)*3.*H(I)**2
      TEMP(2) = AMIN1(TEMP(2),TEMP(3))
 1172 TEMP(2) = AMIN1(TEMP(1), TEMP(2))
      TEMP(2) = TEMP(2)*TELM(25)
C
C             FIND MINIMUM TIME STEP                                    DRAD1680
C
      IF (TEMP(2)) 1230,1230,1190                                       DRAD1700
 1190 IF (TEMP(2)-DTR1) 1200,1210,1210                                  DRAD1710
 1200 DTR2=DTR1                                                         DRAD1720
      IMN2=IMN1                                                         DRAD1730
      DTR1=TEMP(2)                                                      DRAD1740
      IMN1=I                                                            DRAD1750
      GO TO 1230                                                        DRAD1760
 1210 IF (TEMP(2)-DTR2) 1220,1230,1230                                  DRAD1770
 1220 DTR2=TEMP(2)                                                      DRAD1780
      IMN2=I                                                            DRAD1790
 1230 CONTINUE                                                          DRAD1800
      DTRMIN=DTR1                                                       DRAD1810
      EO=IMN1                                                           DRAD1820
C                                                                       DRAD1830
C             SET UP MINIMUM TIME STEPS BETWEEN EDITS                   DRAD1840
C                                                                       DRAD1850
```

```
      IF (DTR1-TELM(26)) 1240,1250,1250
 1240 TELM(26)=DTR1
      TELM(27)=IMN1
      TELM(28)=DTR2
      TELM(29)=IMN2
      TELM(30)=SOLID(18)+1.0
 1250 CONTINUE
C
C           DETERMINE IF RADIATION OR HYDRO WILL SUBCYCLE
C
      IF(DTRMIN-DTR) 1280,125,1260
 1260 BLANK3=TH+AMIN1(DTRMIN,GR*DTH2)
      IF(S17) 125,1270,125
 1270 S9 = 1.0
      GO TO 125
C
C                 REDUCE TIME STEP
C
 1280 NRAD=ZP1(18)/DTRMIN+1.0
      DTR=ZP1(18)/FLOAT(NRAD)
      IF(NRAD-NTIMES) 125,125,1290
 1290 S1=13.1290
      CALL UNCLE
  125 THTAMX=.025
C***********************************************************************
C
C         CALCULATE GEOMETRY FACTORS AND FIND HIGHEST TEMPERATURE
C
C***********************************************************************
      DO 180 I=IN,IM
      GO TO (132, 134, 136), IALPHA
C
C                 SLABS
C
  132 PDFU(I) = 1. / (C(I+1) - C(I))
      RUC(I+1)=5.0E9 / (C(I+2) - C(I))
      GO TO 138
C
C                 CYLINDERS
C
  134 PDFU(I) = 1. / (C(I+1)**2 - C(I)**2)
      RUC(I+1)=1.0E10 * C(I+1) / (C(I+2) - C(I))
      GO TO 138
C
C                 SPHERES
C
  136 PDFU(I) = 1. / (C(I+1)**3 - C(I)**3)
      RUC(I+1)=1.5E10 * C(I+1)**2 / (C(I+2) - C(I))
  138 IF (THETA(I) .LE. THTAMX)  GO TO 180
      THTAMX=THETA(I)
  180 CONTINUE
      IF (THTAMX .LT. THETA(IB) .AND. GL .GT. 0.)  THTAMX = THETA(IB)
      IF (THTAMX .LT. THETA(IA-1) .AND. GA .GT. 0.) THTAMX = THETA(IA-1)
      GO TO (182, 184, 186), IALPHA
C
C                 BOUNDARY QUANTITIES
C
  182 TSLH = 1.
      TSRH = 1.
      GO TO 188
  184 TSLH = C(IN) + C(IN)
      TSRH = C(IMP1) + C(IMP1)
      GO TO 188
  186 TSLH = 3. * C(IN)**2
      TSRH = 3. * C(IMP1)**2
```

```
  188 CDT = 1.2E11 * DTR
      RCDT = 1. / CDT
      RDTR = 1. / DTR
      CALL DVCHK(KDMY)
      GO TO (190, 200), KDMY
  190 S1 = 13.0190
      CALL UNCLE
C
C             ZERO X3, X4, X5, X6 (IN CASE MERGE FREQUENCIES)
C             AND ER, SUMX2, SUMRHO (FOR FREQUENCY INTEGRATION)
C
  200 DO 210 I=IN,IM
      X3(I)=0.
      X4(I)=0.
      X5(I)=0.
      X6(I)=0.
      ER(I) = 0.
      SUMX2(I) = 0.
      SUMRHO(I) = 0.
C
C             SET UP FOR KAPPA INTERPOLATION
C
  210 Q1(I)=THETA(I)**4
      SUMX2(IMP1) = 0.
C
C
C***********************************************************************
C                                                                      *
C             B E G I N   F R E Q U E N C Y   L O O P                  *
C                                                                      *
C***********************************************************************
C
C             SET UP MAX FREQ BOUNDARY
C
      HNUP=1.0E6
      HNUP4=1.0E24
      IF (KMAX.EQ.0) GO TO 280
  220 IHNU = IHNU +1
      CALL KAPPA(IN,IM)
      HNU4=HNU**4
      DHNUP = DHNU
      DHNU = HNUP - HNU
C
C        MERGE GROUPS WITH HNU MORE THAN CB  TIMES LARGEST THETA
C
C             DON'T KNOW HOW TO MERGE E AND F.  NO MERGE FOR NOW
C
      CB=1.0E10
C
      IF (CB  .GT. 0.0)  GO TO 225
      S1 = 13.0220
      CALL UNCLE
  225 IF  (THETAMX - HNU / CB)  240, 230, 230
  230 IF (IHNU - 1)  235, 370, 260
  235 S1 = 13.0235
      CALL UNCLE
C
C             REJECT TAPE IF MORE THAN HALF OF GROUPS MERGE
C
  240 IF (IHNU+IHNU-NHNU) 260,250,250
  250 IF (AMOD(CB,1.) .EQ. 0.5)  GO TO 260
      S1=13.0250
      CALL UNCLE
  260 DO 270 I=IN,IM
      BETA=HNU/THETA(I)
```

```
      BETAP=HNUP/THETA(I)
      DFB=PLNKUT(BETA,BETAP)
      IF (DFB.EQ.0.) GO TO 270
      TEMP(1)=DFB*Q1(I)
      EMB1=EXP(-BETA)
      EMB2=EXP(-BETAP)
      TEMP(2)=DFB+0.0384974/Q1(I)*(HNU4/(1.0-EMB1)
     I*EMB1-HNUP4/(1.0-EMB2)*EMB2)
C
C              FORM NUMERATORS AND DENOMINATORS OF MERGED KAPPAS
C
      X6(I)=X6(I)+TEMP(1)
      X4(I)=X4(I)+TEMP(2)
      X5(I)=X5(I)+CAPAC(I)*TEMP(1)
      X3(I)=X3(I)+TEMP(2)/CAPAR(I)
  270 CONTINUE
      HNUP=HNU
      HNUP4=HNU4
      IF (THTAMX- HNU/CB) 220,310,310
C
C              FORM MERGED KAPPAS
C
  310 DO 350 I=IN,IM
      IF (X6(I)) 320,350,330
  320 S1=13.0320
      CALL UNCLE
  330 CAPAR(I)=X4(I)/X3(I)
      CAPAC(I)=X5(I)/X6(I)
  350 CONTINUE
      HNUP=1.0E6
      HNUP4=1.0E24
      DHNU = HNUP - HNU
      GO TO 480
C
C              MONOFREQUENCY CALCULATION
C
  280 NHNU=1
        IHNU = 1
      DO 290 I=IN,IM
  290 X6(I)=Q1(I)
      HNU = .001
      GO TO 480
C
C              FREQUENCY GROUP CALCULATION OF SOURCES
C
  360 IHNU = IHNU +1
      CALL KAPPA(IN,IM)
      DHNU=HNUP-HNU
      HNU4=HNU**4
  370 DO  392  I = IN, IM
      DFB = PLNKUT(HNU / THETA(I), HNUP / THETA(I))
  392 X6(I)=DFB*Q1(I)
C
C              SET BOUNDARY CONDITION FOR LEFT HAND SIDE
C
  480 IF (INM1)  490, 510, 500
  490 S1=13.0490
      CALL UNCLE
  500 IF(KMAX .EQ. 0)  GO TO 501
      IF (THETA(INM1) .LE. 0.0) THETA(INM1) = 1.0E-5
      DFB=PLNKUT(HNU/THETA(INM1),HNUP/THETA(INM1))
      GO TO 502
  501 DFB=1.
  502 CONTINUE
      BBSL = DFB * THETA(INM1)**4
```

```
      GO TO 520                                                         DRAD3650
C                                                                       DRAD3660
C                NO BOUNDARY CONDITION FOR GA .GT. 0.0
C                                                                       DRAD3680
  510 IF (GA .GT. 0.0)  GO TO 515                                       DRAD3690
      IF (GA .EQ. 0.0)  BBSL = 0.                                       DRAD3700
      GO TO 520                                                         DRAD3710
  515 S1 = 13.0515                                                      DRAD3720
      CALL UNCLE                                                        DRAD3730
C                                                                       DRAD3740
C                SET BOUNDARY CONDITION FOR RIGHT HAND SIDE
C                                                                       DRAD3760
  520 IF (GL .EQ. 0.0) X6(IMP1)=0.0                                     DRAD3770
      IF (GL.NE.0.5) GO TO 530                                          DRAD3780
      IF (KMAX .NE. 0)  GO TO 522
      DFB = 1.
      GO TO 525
  522 DFB = PLNKUT(HNU / THETA(IMP1), HNUP / THETA(IMP1))               ERAD3790
  525 X6(IMP1) = DFB * THETA(IMP1)**4                                   ERAD3800
C                                                                       DRAD3810
C                SPECIAL RIGHT BOUNDARY SOURCE (GL A POSITIVE            DRAD3820
C                INTEGER) NOW INCLUDED
C                                                                       DRAD3840
  530 IF(GL.GT.0.5) X6(IMP1) = FLUX (IHNU)                              DRAD3850
      BBR=-X6(IMP1)                                                     DRAD3860
C                                                                       DRAD3870
C                FORM ROSSELAND AND PLANCK OPTICAL DEPTHS               DRAD3880
C                                                                       DRAD3890
      H3M = CAPAR(IN) / SV(IN) * DELTAR(IN)                             DRAD3900
      DO 580 I=IN,IM                                                    DRAD3910
      IF (AMIN1(CAPAC(I), CAPAR(I)) .GT. 0.0)  GO TO 560                DRAD3920
      S1=13.0550                                                        DRAD3930
      CALL UNCLE                                                        DRAD3940
C                                                                       DRAD3950
C                FOR NONEQUILIBRIUM DIFFUSION, H AND H2                 DRAD3960
C                ARE MU AND (1./(4.*LAMBDA)) RESPECTIVELY.              DRAD3970
C                                                                       DRAD3980
  560 H(I) = CAPAC(I) / SV(I) * 1.5E10                                  DRAD3990
      IF(SOLID(10).NE.0.0) H(I) = H(I)*CAPAR(I)/CAPAC(I)                DRAD4000
      SU(I) =  2.74E2 * H(I) * X6(I)                                    DRAD4010
      IF (I .EQ. IM)  GO TO 580                                         DRAD4020
C                                                                       DRAD4030
C                WARNING - ASYNCHRONISMS IN SV AND DELTAR LEAD TO       DRAD4040
C                ERRONEOUS FLUCTUATIONS IN H3.  THIS CAN BE FIXED       DRAD4050
C                BY SUBSTITUTING G IN PLANES, BUT SPHERES WILL          DRAD4060
C                STILL HAVE THIS TROUBLE.                               DRAD4070
C                                                                       DRAD4080
  576 H3P = CAPAR(I+1) / SV(I+1) * DELTAR(I+1)                          DRAD4090
C
C     FOR SHARP CHANGES IN OPTICAL DEPTH, USE THINNER ZONE TO DEFINE H2
C
CAVEAT.  TROUBLE IN SCATTERING PROBLEMS - CODE CHANGES SOON
C
      IF(ABS(H3M-H3P)/(H3M+H3P).LE.AC)  GO TO 578                       DRAD4100
       H2(I+1)=.25*AMIN1(H3M/DELTAR(I),H3P/DELTAR(I+1))                 DRAD4110
      GO TO 580                                                         DRAD4120
  578 H2(I+1) = (H3M + H3P) * 0.25/ (DELTAR(I) + DELTAR(I+1))           DRAD4130
  580 H3M = H3P                                                         DRAD4170
C
C                INITIALIZE E SUPER N AND F SUPER N
C
      IF (NVEZ .EQ. 2 .AND. CVB .NE. 0.0)  GO TO 592
      IF (SOLID(18) .GT. 0.0 .AND. LMDA(26) .EQ. 0) GO TO 585
      LMDA(26) = 0
      DO  583  I = IN, IM
```

```
      OLDE(I,IHNU) = 157.0 * X6(I)
  583 OLDF(I,IHNU) = 0.0
      OLDF(IMP1,IHNU) = 0.0
      GO TO 592
  585 IF (SOLID(18) .GT. SCYCLE .OR.   ILMDA .EQ. 12345) GO TO 592
  587 READ (13)  TESTC, (OLDE(I,IHNU), OLDF(I,IHNU), I=1,152)
      IF (IHNU .GT. 1)  GO TO 592
      IF (TESTC - SOLID(18))  587, 592, 590
  590 S1 = 13.0590
      CALL UNCLE
C                                                                       DRAD4180
C                  EXTRAPOLATION COEFFICIENTS TO FORM RADIATION         DRAD4190
C                  ENERGIES AT BOUNDARIES                               DRAD4200
C                                                                       DRAD4210
  592 BETA1 = 1.0 / (2.0 - EXP(-DELTAR(IN) * SQRT(CAPAR(IN) * H(IN) *
     2 5.0E-11 / SV(IN))))
      BETA2 = 1.0 / (2.0 - EXP(-DELTAR(IM) * SQRT(CAPAR(IM) * H(IM) *
     2 5.0E-11 / SV(IM))))
      CALL DVCHK(KDMY)
      GO TO (588, 589), KDMY
  588 S1 = 13.0588
      CALL UNCLE
C***********************************************************************DRAD4260
C                                                                       DRAD4270
C                    NONEQUILIBRIUM DIFFUSION TREATMENT                 DRAD4280
C                                                                       DRAD4290
C                  FORM COEFFICIENTS OF IMPLICIT EQUATIONS              DRAD4300
C                                                                       DRAD4310
C***********************************************************************DRAD4320
C                                                                       DRAD4330
  589 IF(INP1-IM) 593,593,1500                                          DRAD4340
C                                                                       DRAD4350
C                  SPECIAL CASE - SINGLE VAPOR ZONE                     DRAD4360
C                                                                       DRAD4370
 1500 CONTINUE                                                          DRAD4380
      BU = 2.*H(IN) +1.5E10*(TSRH*BETA2 +TSLH*BETA1)*PDFU(IN)+RDTR
      DU=2.055E12*PDFU(IN)*(BBSL*TSLH*BETA1-BBR*TSRH*BETA2)
     1     +RDTR*OLDE(IN,IHNU)
      IF(KMAX.EQ.0.AND.HVB.NE.0.0)GO TO 1550                            DRAD4410
C                                                                       DRAD4420
C                  PARTIALLY IMPLICIT - MULTIFREQUENCY CASE             DRAD4430
C                                                                       DRAD4440
 1530 CONTINUE                                                          DRAD4450
      RHO(IN)=(SU(IN)+DU)/BU
      GO TO 669                                                         DRAD4480
C                                                                       DRAD4490
C                  FULLY IMPLICIT TERMS                                 DRAD4500
C                                                                       DRAD4510
 1550 GO TO(1595,1596),NVEZ                                             DRAD4520
C                                                                       DRAD4530
C                  NO ITERATION                                         DRAD4540
C                                                                       DRAD4550
 1595 T4=Q1(IN)                                                         DRAD4560
      GO TO 1597                                                        DRAD4570
 1596 IF(CVB.EQ.0.0)GO TO 1595                                          DRAD4580
C                                                                       DRAD4590
C                  ITERATION                                            DRAD4600
C                                                                       DRAD4610
      T4=OLDTH(IN)**4                                                   DRAD4620
 1597 TEMP(1)=5.48E2*THETA(IN)**3                                       DRAD4630
      TEMP(2)=G(IN)*RDTR*CV(IN)                                         DRAD4640
      DENOM=TEMP(2)/H(IN)+TEMP(1)/PDFU(IN)                              DRAD4650
      BU=BU-2.*H(IN)/PDFU(IN)*TEMP(1)/DENOM
      SU(IN) =  (SMLQ(IN) - (PB1(IN) + P(IN)) * VD(IN)) *(TEMP(1)  /    ********
     2 DENOM)- (TEMP(2)/DENOM) * 2.74E2 * T4                            ********
```

```
      GO TO 1530
C
C                 LEFT-HAND BOUNDARY CONDITION
C
  593 QU1 = 1. / (RCDT + H2(IN+1))
      RU1 = RUC(IN+1) * QU1
      CU = -PDFU(IN) * RU1
      BU = RDTR + H(IN) + H(IN)
      DU= -RDTR*OLDE(IN,IHNU)+PDFU(IN)*QU1*RCDT*OLDF(IN+1,IHNU)
      IF (KMAX .EQ. 0   .AND. HVB .NE. 0.0)  GO TO 594
      DU = DU - SU(IN)
      GO TO 598
C
C                 FULLY IMPLICIT TERMS
C
  594 GO TO (595, 596), NVEZ
C
C                 NO ITERATION
C
  595 T4 = Q1(IN)
      GO TO 597
  596 IF (CVB .EQ. 0.0)  GO TO 595
C
C                 ITERATION
C
      T4 = OLDTH(IN)**4
  597 TEMP(1) = 5.48E2 * THETA(IN)**3
      TEMP(2) = G(IN) * RDTR * CV(IN)
      DENOM = TEMP(2) / H(IN) + TEMP(1) / PDFU(IN)
      BU = BU -2.*H(IN)/PDFU(IN) * TEMP(1) / DENOM
      DU = DU -  (SMLQ(IN) - (PB1(IN) +
     2 P(IN)) * VD(IN)) *(TEMP(1)  / DENOM)- (TEMP(2)/DENOM)*2.74E2*T4
  598 IF (INM1)  490, 600, 610
  600 IF (GA .LT. 0.0)  GO TO 620
  610 TS1 = PDFU(IN) * TSLH * 1.5E10 * BETA1
      BU = BU + TS1
      DU = DU - TS1 * 137.0 * BBSL
  620 GU(IN) = BU / (CU - BU)
      HU(IN) = DU / (CU - BU)
      IF(INP1-IM) 630,650,625
  625 S1 = 13.0625
      CALL UNCLE
C
C                 GENERAL CASE -- FORWARD PASS
C
  630 IMM1 = IM - 1
      DO  640  I = INP1, IMM1
      QU2 = 1. / (RCDT + H2(I+1))
      RU2 = RUC(I+1) * QU2
      AU = -PDFU(I) * RU1
      CU = -PDFU(I) * RU2
      BU = RDTR + H(I) + H(I)
      DU = -RDTR * OLDE(I,IHNU) + PDFU(I) * RCDT *(QU2 * OLDF(I+1,IHNU)
     1  -QU1 * OLDF(I,IHNU))
      IF (KMAX .EQ. 0   .AND. HVB .NE. 0.0)  GO TO 634
      DU = DU - SU(I)
      GO TO 638
C
C                 FULLY IMPLICIT TERMS
C
  634 GO TO (635, 636), NVEZ
C
C                 NO ITERATION
C
  635 T4 = Q1(I)
```

```
      GO TO 637
  636 IF (CVB .EQ. 0.0)  GO TO 635
C
C                 ITERATION
C
      T4 = OLDTH(I)**4
  637 TEMP(1) = 5.48E2 * THETA(I)**3
      TEMP(2) = G(I ) * RDTR * CV(I )
      DENOM = TEMP(2) / H(I ) + TEMP(1) / PDFU(I)
      BU = BU -2.*H(I)/ PDFU(I ) * TEMP(1) / DENOM
      DU = DU -  ( SMLQ(I) - (PB1(I) +
     2 P(I)) * VD(I)) *(TEMP(1)  / DENOM)- (TEMP(2)/DENOM) * 2.74E2 * T4
  638 DENOM = BU - CU + AU*GU(I-1)
      GU(I) = (-BU - AU*GU(I-1)) / DENOM
      HU(I) = -(DU + AU * HU(I-1)) / DENOM
      QU1 = QU2
      RU1 = RU2
  640 CONTINUE
C
C                 RIGHT-HAND BOUNDARY CONDITION
C
  650 AU = -PDFU(IM) * RU1
      BU = RDTR + H(IM) + H(IM)
      DU = -RDTR * OLDE(IM,IHNU) - PDFU(IM) * RCDT * QU1 * OLDF(IM,IHNU)
      IF (KMAX .EQ. 0    .AND. HVB .NE. 0.0)  GO TO 654
      DU = DU - SU(IM)
      GO TO 658
C
C                 FULLY IMPLICIT TERMS
C
  654 GO TO (655, 656), NVEZ
C
C                 NO ITERATION
C
  655 T4 = Q1(IM)
      GO TO 657
  656 IF (CVB .EQ. 0.0)  GO TO 655
C
C                 ITERATION
C
      T4 = OLDTH(IM)**4
  657 TEMP(1) = 5.48E2 * THETA(IM)**3
      TEMP(2) = G(IM) * RDTR * CV(IM)
      DENOM = TEMP(2) / H(IM) + TEMP(1) / PDFU(IM)
      BU = BU -2.*H(IM)/PDFU(IM) * TEMP(1) / DENOM
      DU = DU - (SMLQ(IM) - (PB1(IM) +
     2 P(IM)) * VD(IM)) *(TEMP(1)  / DENOM)- (TEMP(2)/DENOM)*2.74E2*T4
  658 IF (GL .LT. 0.)  GO TO 660
      TS1 = PDFU(IM) * TSRH * 1.5E10 * BETA2
      BU = BU + TS1
      DU = DU + TS1 * 137.0 * BBR
  660 GU(IM) = -1.
      HU(IM) = -(DU + AU * HU(IM-1)) / (BU + AU * GU(IM-1))
C**********************************************************************
C
C          FORM RADIATION ENERGY, FLUX AND RADIATION SOURCE ER.
C
C**********************************************************************
      DO  670  I = IN, IM
      IBK = IN + IM - I
      RHO(IBK) = (GU(IBK) + 1.) * RHO(IBK+1) + HU(IBK)
      IF (RHO(IBK) .GE. 0.0)  GO TO 670
      S1 = 13.0669
      CALL UNCLE
  670 CONTINUE
```

```
C                                                                        DRAD5950
C                   CHECK ON BOUNDARY X2'S BYPASSED FOR NOW              DRAD5960
C                                                                        DRAD5970
  669 IF(INM1)490,671,673                                                DRAD5980
  671 IF (GA)  672, 673, 673                                             DRAD5990
  672 X2(IN) = 0.0                                                       DRAD6000
      GO TO 674                                                          DRAD6010
  673 X2(IN) = (2.055E12*BBSL -1.5E10*RHO(IN))*TSLH*BETA1
  674 IF(GL)675,678,678                                                  DRAD6030
  675 X2(IMP1) = 0.0                                                     DRAD6040
      GO TO 679                                                          DRAD6050
  678 X2(IMP1) = (2.055E12*BBR +1.5E10*RHO(IM))*TSRH*BETA2
      IF(IM-INP1)700,679,679                                             DRAD6070
C                                                                        DRAD6080
C                   FORM FLUXES                                          DRAD6090
C                                                                        DRAD6100
  679 DO  680  I = INP1, IM                                              DRAD6110
  680 X2(I) = (RCDT * OLDF(I,IHNU) + RUC(I) * (HU(I-1)
     1  + GU(I-1) * RHO(I))) / (RCDT + H2(I))
      CALL DVCHK(KDMY)                                                   DRAD6130
      GO TO (690, 700), KDMY                                             DRAD6140
  690 S1 = 13.0690                                                       DRAD6150
      CALL UNCLE                                                         DRAD6160
C                                                                        DRAD6170
C                   FORM RADIATION CONTRIBUTION TO ZONE ENERGY           DRAD6180
C                                                                        DRAD6190
  700 DO  710  I =IN, IM                                                 DRAD6200
      ER(I)=ER(I)+X2(I)-X2(I+1)+RDTR/PDFU(I)*(OLDE(I,IHNU)-RHO(I))
      GO TO (710, 704), NVEZ
  704 OLDE(I,IHNU) = RHO(I)
      OSX2(I) = OSX2(I) + OLDF(I,IHNU)
      OLDF(I,IHNU) = X2(I)
  710 CONTINUE                                                           DRAD6220
      IF (NVEZ .NE. 2)  GO TO 990
      OSX2(IMP1) = OSX2(IMP1) + OLDF(IMP1,IHNU)
      OLDF(IMP1,IHNU) = X2(IMP1)
C*************************************************************************
C                                                                        DRAD6230
C                   OPTIONAL EDIT OF X2 ETC.                             DRAD6240
C                                                                        DRAD6250
C*************************************************************************
  990 CNT1=SOLID(18)+1.0                                                 DRAD6260
      CNT2=AMIN1(TPRINT,CNTMAX)                                          DRAD6270
      IF (CNT1 .LT. CNT2) GO TO 1020                                     DRAD6280
      F (SOLID(18) .EQ. SCYCLE .OR. NVEZ .EQ. 1
     1               .OR. (ZP1(18)/DTR) .GT. 1.5)  GO TO 1000
      WRITE (13)        CNT1, (OLDE(I,IHNU), OLDF(I,IHNU), I=1,152)
 1000 IF (EDITMF .EQ. 0.0) GO TO 1020                                    DRAD6290
      TEMP(1) = TH + DTR                                                 DRAD6300
      WRITE (6,3) CNT1, TEMP(1), HNU, NVEZ
      WRITE (6,4)
      H(IMP1) = 0.
      H2(IMP1) = 0.
      GU(IMP1) = 0.
      HU(IMP1) = 0.
      RHO(IMP1) = 0.
      DO 1010 I = IN, IMP1
 1010 WRITE (6,5) I,THETA(I),X6(I),H(I),H2(I),GU(I),HU(I),RHO(I),X2(I)
    3 FORMAT  (9H1CYCLE = F7.0, 9H  TIME = E13.6, 4X11HHNU(LOWER)=F10.4,
     2 10H PASS NO. I1/)
    4 FORMAT  (7X1HI, 9X5HTHETA, 12X2HX6, 13X1HH, 12X2HH2, 12X2HGU,
     2 12X2HHU, 11X3HRHO, 12X2HX2)
    5 FORMAT  (I8, 1P8E14.7)
C                                                                        DRAD6390
C     ADVANCE FREQ, STORE EMERGENT FLUX, TEST FOR COMPLETION OF GROUPS   DRAD6400
```

```
C                                                                       DRAD6410
 1020 DO 1030 I=IN,IMP1                                                 DRAD6420
      SUMRHO(I) = SUMRHO(I) + RHO(I)                                    DRAD6430
      SUMX2(I)=SUMX2(I)+X2(I)                                           DRAD6440
 1030 CONTINUE                                                          DRAD6450
      CALL DVCHK (K000FX)                                               DRAD6460
      GO TO (1050,1040), K000FX                                         DRAD6470
 1040 IF (IHNU .GT. IDMHNU)  GO TO 1050
      HNUP=HNU                                                          DRAD6490
      HNUP4=HNU4                                                        DRAD6490
      IF(IHNU-NHNU)360,1060,1050                                        DRAD6500
C***********************************************************************DRAD6510
C                                                                      *DRAD6520
C                  E N D   F R E Q U E N C Y   L O O P                 *DRAD6530
C                                                                      *DRAD6540
C***********************************************************************DRAD6550
 1050 S1 = 13.1050                                                      DRAD6560
      CALL UNCLE                                                        DRAD6570
C                                                                       DRAD6580
C                ITERATE ON TEMPERATURE IF NVEZ EQUALS ONE              DRAD6590
C                                                                       DRAD6600
 1060    ILMDA=12345
      GO TO (1061, 1065), NVEZ
 1061 NVEZ = 2                                                          DRAD6620
      VEZ = NVEZ                                                        DRAD6630
      NY = NVEZ                                                         DRAD6640
      IHNU=0                                                            DRAD6650
      DO  1062  I = IN, IM                                              DRAD6660
      BNTH = THETA(I) + (SMLQ(I) + ER(I) - (PB1(I) + P(I)) * VD(I)) *   DRAD6670
     2 DTR / (G(I) * CV(I))                                             DRAD6680
      OLDTH(I) = THETA(I)                                               DRAD6690
      THETA(I) = 0.5 * (OLDTH(I) + BNTH)                                DRAD6700
 1062 Q37(I)=ALOG(THETA(I))                                             DRAD6710
      IF (KMAX.EQ. 0) CALL KAPPA(IN,IM)                                 DRAD6720
      GO TO 200                                                         DRAD6730
 1065 IF (CVB .EQ. 0.0)  GO TO 1067                                     DRAD6740
      DO  1066 I = IN, IM                                               DRAD6750
 1066 THETA(I) = OLDTH(I)                                               DRAD6760
C                                                                       DRAD6770
C                SET UP FOR ENCALC                                      DRAD6780
C                                                                       DRAD6790
 1067 DO  1070  I = IN, IMP1                                            DRAD6800
      Q1(I) = 0.                                                        DRAD6810
      RHO(I) = SUMRHO(I)                                                DRAD6820
 1070 X2(I) = SUMX2(I)                                                  DRAD6830
 1300 IF (ZP1(26) .EQ. 0.0)  GO TO 1400                                 DRAD6840
C                                                                       DRAD6850
C                RESTORE NONEC QUANTITIES
C                                                                       DRAD6870
      IF (PUSHA .LT. 0.0)  GO TO 1350                                   DRAD6880
      CALL NONEQ(IMP1,5)                                                DRAD6890
      GO TO 1400                                                        DRAD6900
 1350 CALL NONEQ(INM1,5)                                                DRAD6910
 1400 RETURN                                                            DRAD6920
      END                                                               DRAD6921
```

```
      SUBROUTINE  RADTN
C***********************************************************************
C
C*                  S P U T T E R   C O M M O N                      **
C                                                                     *
      COMMON    LMDA(37), NR     , NSMLR , IA     , IB     , ICA    , ICB    ,
     1   KMAX   , BLANK1, BLANK2, BLANK3, IAP1   , IBP1   , ICAP1  , ICBP1  ,
     2   II     , IG     , NRAD   , BLANK4, IAM1   , IBM1   , ICAM1  , ICPM1  ,
     3   IIP1   , IGM1   , IALPHA, BLANK5, TH     , TMAX   , BLANK6, DELPRT,
     4   FREQ   , CNTMAX, AR     , ASMLR  , PUSHA  , PUSHB  , BOILA  , FOILB  ,
     5   CVA    , CVB    , SLUG   , ALPHA  , HVA    , HVB    , HCA    , HCB    ,
     6   EMINA  , EMINB  , CA     , CB     , GA     , GB     , GL     , GR     ,
      COMMON       TD     , TE     , DTH2   , DTH2P  , DTH1   , DTRMIN, DTMAX  ,
     1   DTMAX1, DTMAX2, DTMAX3, DTR    , SWITCH, CO     , CMIN   , DELTA  ,
     2   GAMA   , WCRIT  , SIGMAQ, AC     , ACO3T4, CNVRT  , SUMRA  , SUMRB  ,
     3   ROIA   , ROIAM1, ROIB   , ROIBP1, GMS    , S1     , S2     , S3     ,
     4   S4     , S5     , S6     , S7     , S8     , S9     , S10    , S11    ,
     5   S12    , S13    , S14    , S15    , S16    , S17    , S18    , S19    ,
     6   S20    , EO     , FO     , TAU    , ZERO   , R      (152), DELTAR(152),
     7  ASQ     (152), RD      (152), VD      (152), RDD     (152), SMLR   (152),
     8  DELR    ( 37), P       (152), P1      (152), PB      (152), PB1    (152)
      COMMON          P2      (152), SV      (152), RHO     (152), THETA  (152),
     1  W       (152), E       (152), EI      (152), EK      (152), A      (152),
     2  V       (152), G       (152), D       (152), C       (152), X2     (152),
     3  X3      (152), X4      (152), X5      (152), X6      (152), X7     (152),
     4  SMLA    (152), SMLB    (152), SMLC    (152), SMLD    (152), SMLE   (152),
     5  EC      (152), EK      (152), SMLQ    (152), SMLH    (152), BIGA   (152),
     6  BIGB    (152), CV      (152), BC      (152), BR      (152), CHIC   (152),
     7  CHIR    (152), CAPAC (152), CAPAR (152), CRTC    (152), CRTR   (152),
     8  CRTPC (152), GOFR    (152), FEH     (152), CAR     (152), OKLM   ( 37)
      COMMON          TELM    ( 37), EKLM    ( 37), ELM     ( 37), FCLM   ( 37),
     1  FRLM    ( 37), WLM     ( 37), QLM     ( 37), AMASNO( 37), CHRNO  ( 37),
     2  ZP1     ( 37), ZP2     ( 37), SOLID ( 37), ECHCK ( 37), RK     (104),
     3  RL      ( 37), RHOK    (104), RDK     (104), THETAK(104), TEMP   ( 16)
     4  HEAD    ( 12), MAXL          , MAXLM
C*                                                                   **
C***********************************************************************
C
      DIMENSION  RUC(1), OSX2(1), H2(1), Q1(1), GU(1), SU(1), HU(1)
      DIMENSION  PDFU(1), SUMRHO(1), H(1), SUMX2(1), OLDTH(1)
      DIMENSION  Q37(1), Q38(1)
      COMMON /LINDLY/ HNU,SGNL,IHNU,NHNU,HNUP,NT,IM,IN,DHNU,THICK,NY
      COMMON/TQ/QINT1(300),QINT2(300),TITLE(12),FLUX(30)
      COMMON /CNTRL/ SCYCLE, JMULT
C
      EQUIVALENCE  (SMLA,PDFU), (SMLD,SUMRHO)
      EQUIVALENCE  (BC,OSX2),(BIGB,H),(CRTR,SUMX2),(CHIC,SU)
      EQUIVALENCE  (SMLH,GU),(CAR,Q37),(CHIR,Q38),(SMLC,OLDTH)
      EQUIVALENCE  (ACO3T4,TRDBG),(S12,EDITMF)
      EQUIVALENCE (EC,Q1),(X7,H2),(BIGA,HU    ),(GOFR,RUC)
C
C**********************************************************************
C                                                                    *
C                     EDITMF SAME AS     S12                         *
C                     H      SAME AS    BIGB                         *
C                     H2     SAME AS      X7                         *
C                     OLDTH  SAME AS    SMLC                         *
C                     PDFU   SAME AS    SMLA                         *
C                     Q1     SAME AS      EC                         *
C                     RUC    SAME AS    GOFR                         *
C                     Q37    SAME AS     CAR                         *
C                     Q38    SAME AS    CHIR                         *
C                     SUMX2  SAME AS    CRTR                         *
C                     SU     SAME AS    CHIC                         *
C                     HU     SAME AS    BIGA                         *
C                     TRDBG  SAME AS  ACO3T4                         *
```

```
C                              GU      SAME AS    SMLH
C                              SUMRHO SAME AS    SMLD
C
C***********************************************************************
C
C     NONEQUILIBRIUM RADIATION DIFFUSION AS IN LA-3377
C
C     FOR DRADTN AND ERADTN. NY (IN LINDLEY COMMON) IS TEMPERATURE
C     ITERATION INDEX.  THIS IS USED IN A SPECIAL DIANA THAT GOES WITH
C     DRADTN AND ERADTN.
C
C***********************************************************************
C
C          INITIALIZATION AND CALCULATION FOR NO VAPOR ZONES
C
C***********************************************************************
C
      CALL DVCHK (K000FX)
      NTIMES=BOILB
      IM=IBM1
      IN=IA
      IF (KMAX .EQ. 0)  DHNU = 1.
   10 IF (ZP1(26).EQ.0.) GO TO 30
C
C               SAVE STUFF FROM EIONX FOR NONEQ AND RESET IN OR IM
C
      IF (PUSHA.LT.0.0) GO TO 20
      IM = NR - 1
      CALL NONEQ(IM+1,4)
      GO TO 30
   20 IN = NR
      CALL NONEQ(IN-1,4)
   30 CONTINUE
      IMP1=IM+1
      INM1=IN-1
      INP1 = IN + 1
   40 IF (IMP1-IN) 50,50,60
C
C         CALCULATE BLACKBODY EMISSION AND EXIT IF NO VAPOR ZONES
C
   50 X2(IMP1) = 1.0275E12 * A(IMP1) * (THETA(IM)**4 - THETA(IMP1)**4)
      ER(IM)=-X2(IMP1)
      GO TO 1310
   60 NVEZ = 1
      NY = NVEZ
      IF(CVB.EQ.0.0) NVEZ = 2
      VEZ = NVEZ
C
C         FORM INTERPOLATION QUANTITIES FOR OPACITY SUBROUTINE
C
      DO 70 I=IN,IM
      Q37(I)=ALOG(THETA(I))
   70 Q38(I)=ALOG(SV(I))
C
C        OBTAIN ROSSELAND AND PLANCK OPACITIES FOR ENTIRE SPECTRUM
C        (REQUIRES DIANE TAPE HAVING MONOFREQUENCY OPACITIES FIRST)
C
      IHNU = 0
      CALL KAPPA(IN,IM)
C***********************************************************************
C
C        M I N I M U M   T I M E   S T E P   C A L C U L A T I O N
C
C***********************************************************************
      WSB = 0.0
```

```
      DO 80 I=1,MAXLM
   80 WSB = WSB + ELM(I)
      DTR1=1.E10
      DTR2=1.E10
   90 DO 210 I=IN,IM
C
C                CALL UNCLE IF EITHER KAPPA IS ZERO OR NEGATIVE
C
      IF (AMIN1(CAPAC(I),CAPAR(I)).GT.0.0) GO TO 100
   95 S1=13.0095
      CALL UNCLE
C
C                SOLID(10) NOT ZERO GIVES ALL ROSSELAND OPTION
C
  100 IF (SOLID(10).EQ.0.0) GO TO 110
      TEMP(1) = CAPAR(I)
      TEMP(3) = CAPAR(I)
      GO TO 120
  110 TEMP(1)=SQRT(CAPAR(I)*CAPAC(I))
      TEMP(3) = CAPAC(I)
  120 IF (0.001-THETA(I)) 130,210,210
  130 H(I) = 0.5 * TEMP(1) / SV(I) * DELTAR(I)
      TEMP(1) = 1.E10
      TEMP(2) = 1.E10
      IF (TELM(37).EQ.0.0.OR.ER(I).EQ.0.0) GO TO 150
      WSBB = E(I) * G(I)
      IF (WSBB-TELM(37)*WSB) 150,140,140
C
C     ACCURACY CRITERION - DONE FOR FULLY AND PARTIALLY IMPLICIT CASES
C
  140 TEMP(1) = SLUG * WSBB / ABS(ER(I))
  150 IF (KMAX.EQ.0.AND.HVB.NE.0.0) GO TO 160
C
C              STABILITY CRITERION -- BYPASSED IN FULLY IMPLICIT CASE
C
      TEMP(2) = .5*CV(I)/(4.1132E12*TEMP(3)*THETA(I)**3)
      TEMP(3) = TEMP(2)*3.*H(I)**2
      TEMP(2) = AMIN1(TEMP(2),TEMP(3))
  160 TEMP(2) = AMIN1(TEMP(1), TEMP(2))
      TEMP(2)=TEMP(2)*TELM(25)
C
C                FIND MINIMUM TIME STEP
C
      IF (TEMP(2)) 210,210,170
  170 IF (TEMP(2)-DTR1) 180,190,190
  180 DTR2=DTR1
      IMN2=IMN1
      DTR1=TEMP(2)
      IMN1=I
      GO TO 210
  190 IF (TEMP(2)-DTR2) 200,210,210
  200 DTR2=TEMP(2)
      IMN2=I
  210 CONTINUE
      DTRMIN=DTR1
      EO=IMN1
C
C               SET UP MINIMUM TIME STEPS BETWEEN EDITS
C
      IF (DTR1-TELM(26)) 220,230,230
  220 TELM(26)=DTR1
      TELM(27)=IMN1
      TELM(28)=DTR2
      TELM(29)=IMN2
      TELM(30)=SOLID(18)+1.0
```

```
  230 CONTINUE
C
C          DETERMINE IF RADIATION OR HYDRO WILL SUBCYCLE
C
      IF (DTRMIN-DTR) 260,280,240
  240 BLANK3=TH+AMIN1(DTRMIN,GR*DTH2)
      IF (S17) 280,250,280
  250 S9 = 1.0
      GO TO 280
C
C               REDUCE TIME STEP
C
  260 NRAD=ZP1(18)/DTRMIN+1.0
      DTR=ZP1(18)/FLOAT(NRAD)
      IF (NRAD-NTIMES) 280,280,270
  270 S1=13.0270
      CALL UNCLE
  280 THTAMX=.025
C***********************************************************************
C
C          CALCULATE GEOMETRY FACTORS AND FIND HIGHEST TEMPERATURE
C
C***********************************************************************
      DO 330 I=IN,IM
      GO TO (290,300,310), IALPHA
C
C               SLABS
C
  290 PDFU(I) = 1. / (C(I+1) - C(I))
      RUC(I+1)=5.0E9 / (C(I+2) - C(I))
      GO TO 320
C
C               CYLINDERS
C
  300 PDFU(I) = 1. / (C(I+1)**2 - C(I)**2)
      RUC(I+1)=1.0E10 * C(I+1) / (C(I+2) - C(I))
      GO TO 320
C
C               SPHERES
C
  310 PDFU(I) = 1. / (C(I+1)**3 - C(I)**3)
      RUC(I+1)=1.5E10 * C(I+1)**2 / (C(I+2) - C(I))
  320 IF (THETA(I).LE.THTAMX) GO TO 330
      THTAMX=THETA(I)
  330 CONTINUE
      IF (THTAMX .LT. THETA(IB) .AND. GL .GT. 0.)  THTAMX = THETA(IB)
      IF (THTAMX .LT. THETA(IA-1) .AND. GA .GT. 0.) THTAMX = THETA(IA-1)
      GO TO (340,350,360), IALPHA
C
C               BOUNDARY QUANTITIES
C
  340 TSLH = 1.
      TSRH = 1.
      GO TO 370
  350 TSLH = C(IN) + C(IN)
      TSRH = C(IMP1) + C(IMP1)
      GO TO 370
  360 TSLH = 3. * C(IN)**2
      TSRH = 3. * C(IMP1)**2
  370 RDTR = 1. / DTR
      CALL DVCHK(KDMY)
      GO TO (380,390), KDMY
  380 S1 = 13.0380
      CALL UNCLE
C
```

```
C               ZERO X3, X4, X5, X6 (IN CASE MERGE FREQUENCIES)
C               AND ER, SUMX2, SUMRHO (FOR FREQUENCY INTEGRATION)
C
  390 DO 400 I=IN,IM
      X3(I)=0.
      X4(I)=0.
      X5(I)=0.
      X6(I)=0.
      ER(I) = 0.
      SUMX2(I) = 0.
      SUMRHO(I) = 0.
C
C               SET UP FOR KAPPA INTERPOLATION
C
  400 Q1(I)=THETA(I)**4
      SUMX2(IMP1) = 0.
C
C
C**********************************************************************
C                                                                     *
C               B E G I N   F R E Q U E N C Y   L O O P               *
C                                                                     *
C**********************************************************************
C
C               SET UP MAX FREQ BOUNDARY
C
      HNUP=1.0E6
      HNUP4=1.0E24
      IF (KMAX.EQ.0) GO TO 530
  410 IHNU = IHNU +1
      CALL KAPPA(IN,IM)
      HNU4=HNU**4
      DHNUP = DHNU
      DHNU = HNUP - HNU
C
C          MERGE GROUPS WITH HNU MORE THAN CB  TIMES LARGEST THETA
C
      IF (CB.GT.0.0) GO TO 420
  415 S1 = 13.0415
      CALL UNCLE
  420 IF (THTAMX-HNU/CB) 450,430,430
  430 IF (IHNU-1) 440,560,470
  440 S1 = 13.0440
      CALL UNCLE
C
C               REJECT TAPE IF MORE THAN HALF OF GROUPS MERGE
C
  450 IF (IHNU+IHNU-NHNU) 470,460,460
  460 IF (AMOD(CB,1.).EQ.0.5) GO TO 470
      S1=13.0460
      CALL UNCLE
  470 DO 480 I=IN,IM
      BETA=HNU/THETA(I)
      BETAP=HNUP/THETA(I)
      DFB=PLNKUT(BETA,BETAP)
      IF (DFB.EQ.0.) GO TO 480
      TEMP(1)=DFB*Q1(I)
      EMB1=EXP(-BETA)
      EMB2=EXP(-BETAP)
      TEMP(2)=DFB+0.0384974/Q1(I)*(HNU4/(1.0-EMB1)
     1*EMB1-HNUP4/(1.0-EMB2)*EMB2)
C
C               FORM NUMERATORS AND DENOMINATORS OF MERGED KAPPAS
C
      X6(I)=X6(I)+TEMP(1)
```

```
      X4(I)=X4(I)+TEMP(2)                                               ERAD3260
      X5(I)=X5(I)+CAPAC(I)*TEMP(1)                                      ERAD3270
      X3(I)=X3(I)+TEMP(2)/CAPAR(I)                                      ERAD3280
  480 CONTINUE                                                          ERAD3290
      HNUP=HNU                                                          ERAD3300
      HNUP4=HNU4                                                        ERAD3310
      IF (THTAMX-HNU/CB) 410,490,490                                    ERAD3320
C                                                                       ERAD3330
C                    FORM MERGED KAPPAS                                 ERAD3340
C                                                                       ERAD3350
  490 DO 520 I=IN,IM                                                    ERAD3360
      IF (X6(I)) 500,520,510                                            ERAD3370
  500 S1=13.0500                                                        ERAD3380
      CALL UNCLE                                                        ERAD3390
  510 CAPAR(I)=X4(I)/X3(I)                                              ERAD3400
      CAPAC(I)=X5(I)/X6(I)                                              ERAD3410
  520 CONTINUE                                                          ERAD3420
      HNUP=1.0E6                                                        ERAD3430
      HNUP4=1.0E24                                                      ERAD3440
      DHNU = HNUP - HNU                                                 ERAD3450
      GO TO 580                                                         ERAD3460
C                                                                       ERAD3470
C                    MONOFREQUENCY CALCULATION                          ERAD3480
C                                                                       ERAD3490
  530 NHNU=1                                                            ERAD3500
       IHNU = 1                                                         ERAD3510
      DO 540 I=IN,IM                                                    ERAD3520
  540 X6(I)=Q1(I)                                                       ERAD3530
      HNU = .001                                                        ERAD3540
      GO TO 580                                                         ERAD3550
C                                                                       ERAD3560
C                    FREQUENCY GROUP CALCULATION OF SOURCES             ERAD3570
C                                                                       ERAD3580
  550 IHNU = IHNU +1                                                    ERAD3590
      CALL KAPPA(IN,IM)                                                 ERAD3600
      DHNU=HNUP-HNU                                                     ERAD3610
      HNU4=HNU**4                                                       ERAD3620
  560 DO 570 I=IN,IM                                                    ERAD3630
      DFB = PLNKUT(HNU / THETA(I), HNUP / THETA(I))                     ERAD3640
  570 X6(I)=DFB*Q1(I)                                                   ERAD3650
C                                                                       ERAD3660
C                    SET BOUNDARY CONDITION FOR LEFT HAND SIDE          ERAD3670
C                                                                       ERAD3680
  580 IF (INM1) 590,630,600                                             ERAD3690
  590 S1=13.0590                                                        ERAD3700
      CALL UNCLE                                                        ERAD3710
  600 IF (KMAX.NE.0) GO TO 610                                          ERAD3720
      DFB = 1.                                                          ERAD3730
      GO TO 620                                                         ERAD3740
  610 IF (THETA(INM1) .LE. 0.0) THETA(INM1) = 1.0E-5                    ERAD3750
      DFB = PLNKUT (HNU/THETA(INM1),HNUP/THETA(INM1))                   ERAD3760
  620 BBSL = DFB * THETA(INM1)**4                                       ERAD3770
      GO TO 650                                                         ERAD3780
C                                                                       ERAD3790
C                    NO BOUNDARY CONDITION FOR GA .GT. 0.0              ERAD3800
C                                                                       ERAD3810
  630 IF (GA.GT.0.0) GO TO 640                                          ERAD3820
      IF (GA .EQ. 0.0)  BBSL = 0.                                       ERAD3830
      GO TO 650                                                         ERAD3840
  640 S1 = 13.0640                                                      ERAD3850
      CALL UNCLE                                                        ERAD3860
C                                                                       ERAD3870
C                    SET BOUNDARY CONDITION FOR RIGHT HAND SIDE         ERAD3880
C                                                                       ERAD3890
  650 IF (GL .EQ. 0.0) X6(IMP1)=0.0                                     ERAD3900
```

```
      IF (GL.NE.0.5) GO TO 680
      IF (KMAX.NE.0) GO TO 660
      UFB = 1.
      GO TO 670
  660 UFB = PLNKUT(HNU / THETA(IMP1), HNUP / THETA(IMP1))
  670 X6(IMP1) = UFB * THETA(IMP1)**4
C
C               SPECIAL RIGHT BOUNDARY SOURCE (GL A POSITIVE
C               INTEGER) NOW INCLUDED
C
  680 IF(GL.GT.0.5) X6(IMP1) = FLUX (IHNU)
      BBR=-X6(IMP1)
C
C               FORM ROSSELAND AND PLANCK OPTICAL DEPTHS
C
      H3M = CAPAR(IN) / SV(IN) * DELTAR(IN)
      DO 720 I=IN,IM
      IF (AMIN1(CAPAC(I),CAPAR(I)).GT.0.0) GO TO 690
  685 S1=13.0685
      CALL UNCLE
C
C               FOR NONEQUILIBRIUM DIFFUSION, H AND H2
C               ARE MU AND (1./(4.*LAMBDA)) RESPECTIVELY.
C
  690 H(I) = CAPAC(I) / SV(I) * 1.5E10
      IF(SOLID(10).NE.0.0) H(I) = H(I)*CAPAR(I)/CAPAC(I)
      SU(I) =  2.74E2 * H(I) * X6(I)
      IF (I.EQ.IM) GO TO 720
C
C               WARNING - ASYNCHRONISMS IN SV AND DELTAR LEAD TO
C               ERRONEOUS FLUCTUATIONS IN H3.  THIS CAN BE FIXED
C               BY SUBSTITUTING G IN PLANES, BUT SPHERES WILL
C               STILL HAVE THIS TROUBLE.
C
  700 H3P = CAPAR(I+1) / SV(I+1) * DELTAR(I+1)
C
C     FOR SHARP CHANGES IN OPTICAL DEPTH, USE THINNER ZONE TO DEFINE H2
C
CAVEAT.  TROUBLE IN SCATTERING PROBLEMS - CODE CHANGES SOON
C
      IF (ABS(H3M-H3P)/(H3M+H3P).LE.AC) GO TO 710
       H2(I+1)=.25*AMIN1(H3M/DELTAR(I),H3P/DELTAR(I+1))
      GO TO 720
  710 H2(I+1) = (H3M + H3P) * 0.25/ (DELTAR(I) + DELTAR(I+1))
  720 H3M = H3P
C
C               EXTRAPOLATION COEFFICIENTS TO FORM RADIATION
C               ENERGIES AT BOUNDARIES
C
      BETA1 = 1.0 / (2.0 - EXP(-DELTAR(IN) * SQRT(CAPAR(IN) * H(IN) *
     2 5.0E-11 / SV(IN))))
      BETA2 = 1.0 / (2.0 - EXP(-DELTAR(IM) * SQRT(CAPAR(IM) * H(IM) *
     2 5.0E-11 / SV(IM))))
C*********************************************************************
C
C                    NONEQUILIBRIUM DIFFUSION TREATMENT
C
C               FORM COEFFICIENTS OF IMPLICIT EQUATIONS
C
C*********************************************************************
C
      CALL DVCHK(KDMY)
      GO TO (730,740), KDMY
  730 S1 = 13.0730
      CALL UNCLE
```

```
  740 IF (INP1-IM) 810,810,750
C                                                                       ERAD4560
C                SPECIAL CASE - SINGLE VAPOR ZONE                       ERAD4570
C                                                                       ERAD4580
  750 CONTINUE                                                          ERAD4590
      BU = 2.*H(IN) +1.5E10*(TSRH*BETA2 +TSLH*BETA1)*PDFU(IN)           ERAD4600
      DU=2.055E12*PDFU(IN)*(BBSL*TSLH*BETA1-BBR*TSRH*BETA2)             ERAD4610
      IF (KMAX.EQ.0.AND.HVB.NE.0.0) GO TO 770                           ERAD4620
C                                                                       ERAD4630
C                PARTIALLY IMPLICIT - MULTIFREQUENCY CASE               ERAD4640
C                                                                       ERAD4650
  760 CONTINUE                                                          ERAD4660
      RHO(IN)=(SU(IN)+DU)/BU                                            ERAD4670
      GO TO 1000                                                        ERAD4680
C                                                                       ERAD4690
C                FULLY IMPLICIT TERMS                                   ERAD4700
C                                                                       ERAD4710
  770 GO TO (780,790), NVEZ                                             ERAD4720
C                                                                       ERAD4730
C                NO ITERATION                                           ERAD4740
C                                                                       ERAD4750
  780 T4=Q1(IN)                                                         ERAD4760
      GO TO 800                                                         ERAD4770
  790 IF (CVB.EQ.0.0) GO TO 780                                         ERAD4780
C                                                                       ERAD4790
C                ITERATION                                              ERAD4800
C                                                                       ERAD4810
      T4=OLDTH(IN)**4                                                   ERAD4820
  800 TEMP(1)=5.48E2*THETA(IN)**3                                       ERAD4830
      TEMP(2)=G(IN)*RDTR*CV(IN)                                         ERAD4840
      DENOM=TEMP(2)/H(IN)+TEMP(1)/PDFU(IN)                              ERAD4850
      BU=BU-2.*H(IN)/PDFU(IN)*TEMP(1)/DENOM                             ERAD4860
      SU(IN) =  (SMLQ(IN) - (PB1(IN) + P(IN)) * VD(IN)) *(TEMP(1)  /    ERAD4870
     2 DENOM)- (TEMP(2)/DENOM) * 2.74E2 * T4                            ********
      GO TO 760                                                         ********
C                                                                       ERAD4900
C                LEFT-HAND BOUNDARY CONDITION                           ERAD4910
C                                                                       ERAD4920
  810 RU1=RUC(IN+1)/H2(IN+1)                                            ERAD4930
      CU = -PDFU(IN) * RU1                                              ERAD4940
      BU = H(IN) + H(IN)                                                ERAD4950
      DU = 0.                                                           ERAD4970
      IF (KMAX.EQ.0.AND.HVB.NE.0.0) GO TO 820                           ERAD4980
      UU = DU - SU(IN)                                                  ERAD4990
      GO TO 860                                                         ERAD5000
C                                                                       ERAD5010
C                FULLY IMPLICIT TERMS                                   ERAD5020
C                                                                       ERAD5030
  820 GO TO (830,840), NVEZ                                             ERAD5040
C                                                                       ERAD5050
C                NO ITERATION                                           ERAD5060
C                                                                       ERAD5070
  830 T4 = Q1(IN)                                                       ERAD5080
      GO TO 850                                                         ERAD5090
  840 IF (CVB.EQ.0.0) GO TO 830                                         ERAD5100
C                                                                       ERAD5110
C                ITERATION                                              ERAD5120
C                                                                       ERAD5130
      T4 = OLDTH(IN)**4                                                 ERAD5140
  850 TEMP(1) = 5.48E2 * THETA(IN)**3                                   ERAD5150
      TEMP(2) = G(IN) * RDTR * CV(IN)                                   ERAD5160
      DENOM = TEMP(2) / H(IN) + TEMP(1) / PDFU(IN)                      ERAD5170
      BU = BU -2.*H(IN)/PDFU(IN) * TEMP(1) / DENOM                      ERAD5180
      UU = DU -  (SMLQ(IN) - (PB1(IN) +                                 ********
     2 P(IN)) * VD(IN)) *(TEMP(1)  / DENOM)- (TEMP(2)/DENOM)*2.74E2*T4  ********
```

```
  860 IF (INM1) 590,870,880
  870 IF (GA.LT.0.0) GO TO 890
  880 TS1 = PDFU(IN) * TSLH * 1.5E10 * BETA1
      BU = BU + TS1
      DU = DU - TS1 * 137.0 * BBSL
  890 GU(IN)=BU/(CU-BU)
      HU(IN)=-DU/(BU-CU)
      IF (INP1-IM) 910,980,900
  900 S1 = 13.0900
      CALL UNCLE
C
C                 GENERAL CASE -- FORWARD PASS
C
  910 IMM1 = IM - 1
      DO 970 I=INP1,IMM1
      RU2=RUC(I+1)/H2(I+1)
      AU = -PDFU(I) * RU1
      CU = -PDFU(I) * RU2
      BU = H(I) + H(I)
      DU = 0.
      IF (KMAX.EQ.0.AND.HVB.NE.0.0) GO TO 920
      DU = DU - SU(I)
      GO TO 960
C
C                 FULLY IMPLICIT TERMS
C
  920 GO TO (930,940), NVEZ
C
C                 NO ITERATION
C
  930 T4 = Q1(I)
      GO TO 950
  940 IF (CVB.EQ.0.0) GO TO 930
C
C                 ITERATION
C
      T4 = OLDTH(I)**4
  950 TEMP(1) = 5.48E2 * THETA(I)**3
      TEMP(2) = G(I ) * RDTR * CV(I )
      DENOM = TEMP(2) / H(I ) + TEMP(1) / PDFU(I)
      BU = BU -2.*H(I)/ PDFU(I ) * TEMP(1) / DENOM
      DU = DU -  ( SMLQ(I) - (PB1(I) +
     2 P(I)) * VD(I)) *(TEMP(1)  / DENOM)- (TEMP(2)/DENOM) * 2.74E2 * T4*********
  960 DENOM = BU - CU + AU * GU(I-1)
      GU(I) = (-BU - AU*GU(I-1)) / DENOM
      HU(I) = -(DU + AU * HU(I-1)) / DENOM
      RU1 = RU2
  970 CONTINUE
C
C                 RIGHT-HAND BOUNDARY CONDITION
C
  980 AU = -PDFU(IM) * RU1
      BU=H(IM)+H(IM)
      DU = 0.
      IF (KMAX.EQ.0.AND.HVB.NE.0.0) GO TO 990
      DU = DU - SU(IM)
      GO TO 1030
C
C                 FULLY IMPLICIT TERMS
C
  990 GO TO (1000,1010), NVEZ
C
C                 NO ITERATION
C
 1000 T4 = Q1(IM)
```

```
      GO TO 1020                                                        ERAD5860
 1010 IF (CVB.EQ.0.0) GO TO 1000                                        ERAD5870
C                                                                       ERAD5880
C              ITERATION                                                ERAD5890
C                                                                       ERAD5900
      T4 = OLDTH(IM)**4                                                 ERAD5910
 1020 TEMP(1) = 5.48E2 * THETA(IM)**3                                   ERAD5920
      TEMP(2) = G(IM) * RDTR * CV(IM)                                   ERAD5930
      DENOM = TEMP(2) / H(IM) + TEMP(1) / PDFU(IM)                      ERAD5940
      BU = BU -2.*H(IM)/PDFU(IM) + TEMP(1) / DENOM                      ERAD5950
      DU = DU - (SMLQ(IM) - (PB1(IM) +                                  ********
     2 P(IM)) * VD(IM)) *(TEMP(1)  / DENOM)- (TEMP(2)/DENOM)*2.74E2*T4  ********
 1030 IF (GL.LT.0.) GO TO 1040                                          ERAD5980
      TS1 = PDFU(IM) * TSRH * 1.5E10 * BETA2                            ERAD5990
      BU = BU + TS1                                                     ERAD6000
      DU = DU + TS1 * 137.0 * BBR                                       ERAD6010
 1040 GU(IM) = -1.
      HU(IM) = -(DU+AU*HU(IM-1))/(BU+AU*GU(IM-1))
C***********************************************************************ERAD6040
C                                                                       ERAD6050
C         FORM RADIATION ENERGY, FLUX AND RADIATION SOURCE ER.          ERAD6060
C                                                                       ERAD6070
C***********************************************************************ERAD6080
      DO 1050 I=IN,IM                                                   ERAD6090
      IBK = IN + IM - 1                                                 ERAD6100
      RHO(IBK) = (GU(IBK) + 1.)*RHO(IBK+1) + HU(IBK)
      IF (RHO(IBK).GE.0.0) GO TO 1050                                   ERAD6120
 1045 S1 = 13.1045                                                      ERAD6130
      CALL UNCLE                                                        ERAD6140
 1050 CONTINUE                                                          ERAD6150
C                                                                       ERAD6160
C                 CHECK ON BOUNDARY X2'S BYPASSED FOR NOW               ERAD6170
C                                                                       ERAD6180
 1060 IF (INM1) 590,1070,1090                                           ERAD6190
 1070 IF (GA) 1080,1090,1090                                            ERAD6200
 1080 X2(IN) = 0.0                                                      ERAD6210
      GO TO 1100                                                        ERAD6220
 1090 X2(IN) = (2.055E12*BBSL -1.5E10*RHO(IN))*TSLH*BETA1               ERAD6230
 1100 IF (GL) 1110,1120,1120                                            ERAD6240
 1110 X2(IMP1) = 0.0                                                    ERAD6250
      GO TO 1130                                                        ERAD6260
 1120 X2(IMP1) = (2.055E12*BBR +1.5E10*RHO(IM))*TSRH*BETA2              ERAD6270
      IF (IM-INP1) 1160,1130,1130                                       ERAD6280
C                                                                       ERAD6290
C              FORM FLUXES                                              ERAD6300
C                                                                       ERAD6310
 1130 DO 1140 I=INP1,IM                                                 ERAD6320
 1140 X2(I) = RUC(I)*(HU(I-1)+GU(I-1)*RHO(I))/H2(I)
      CALL DVCHK(KDMY)                                                  ERAD6340
      GO TO (1150,1160), KDMY                                           ERAD6350
 1150 S1 = 13.1150                                                      ERAD6360
      CALL UNCLE                                                        ERAD6370
C                                                                       ERAD6380
C              FORM RADIATION CONTRIBUTION TO ZONE ENERGY               ERAD6390
C                                                                       ERAD6400
 1160 DO 1170 I=IN,IM                                                   ERAD6410
      ER(I) = ER(I) + X2(I) - X2(I+1)                                   ERAD6420
 1170 CONTINUE                                                          ERAD6430
C***********************************************************************ERAD6440
C                                                                       ERAD6450
C              OPTIONAL EDIT OF X2 ETC.                                 ERAD6460
C                                                                       ERAD6470
C***********************************************************************ERAD6480
 1180 CNT1=SOLID(18)+1.0                                                ERAD6490
      CNT2=AMIN1(TPRINT,CNTMAX)                                         ERAD6500
```

```
      IF (CNT1.LT.CNT2) GO TO 1200                                      ERAD6510
 1190 IF (EDITMF.EQ.0.0) GO TO 1200                                     ERAD6520
      TEMP(1) = TH + DTR                                                ERAD6530
      WRITE (6,3) CNT1, TEMP(1), HNU, NVEZ
      WRITE (6,4)
      H(IMP1) = 0.
      H2(IMP1) = 0.
      GU(IMP1) = 0.
      HU(IMP1) = 0.
      RHO(IMP1) = 0.
      DO 1196 I = IN, IMP1
 1196 WRITE (6,5) I,THETA(I),X6(I),H(I),H2(I),GU(I),HU(I),RHO(I),X2(I)
    3 FORMAT  (9H1CYCLE = F7.0, 9H  TIME = E13.6, 4X11HHNU(LOWER)=F10.4,
     2 10H PASS NO. I1/)
    4 FORMAT  (7X1HI, 9X5HTHETA, 12X2HX6, 13X1HH, 12X2HH2, 12X2HGU,
     2 12X2HHU, 11X3HRHO, 12X2HX2)
    5 FORMAT  (I8, 1P8E14.7)
C                                                                       ERAD6620
C     ADVANCE FREQ, STORE EMERGENT FLUX, TEST FOR COMPLETION OF GROUPS  ERAD6630
C                                                                       ERAD6640
 1200 DO 1210 I=IN,IMP1                                                 ERAD6650
      SUMRHO(I) = SUMRHO(I) + RHO(I)                                    ERAD6660
      SUMX2(I)=SUMX2(I)+X2(I)                                           ERAD6670
 1210 CONTINUE                                                          ERAD6680
      CALL DVCHK (K000FX)                                               ERAD6690
      GO TO (1230,1220), K000FX                                         ERAD6700
 1220 HNUP=HNU                                                          ERAD6710
      HNUP4=HNU4                                                        ERAD6720
      IF (IHNU-NHNU) 550,1240,1230                                      ERAD6730
C***********************************************************************ERAD6740
C                                                                      *ERAD6750
C                      E N D   F R E Q U E N C Y   L O O P             *ERAD6760
C                                                                      *ERAD6770
C***********************************************************************ERAD6780
 1230 S1 = 13.1230                                                      ERAD6790
      CALL UNCLE                                                        ERAD6800
C                                                                       ERAD6810
C                ITERATE ON TEMPERATURE IF NVEZ EQUALS ONE              ERAD6820
C                                                                       ERAD6830
 1240 GO TO (1250,1270), NVEZ                                           ERAD6840
 1250 NVEZ = 2                                                          ERAD6850
      VEZ = NVEZ                                                        ERAD6860
      NY = NVEZ                                                         ERAD6870
      IHNU=0                                                            ERAD6880
      DO 1260 I=IN,IM                                                   ERAD6890
      BNTH = THETA(I) + (SMLQ(I) + ER(I) - (PB1(I) + P(I)) * VD(I)) *   ERAD6900
     2 DTR / (G(I) * CV(I))                                             ERAD6910
      OLDTH(I) = THETA(I)                                               ERAD6920
      THETA(I) = 0.5 * (OLDTH(I) + BNTH)                                ERAD6930
 1260 Q37(I)=ALOG(THETA(I))                                             ERAD6940
      IF (KMAX.EQ. 0) CALL KAPPA(IN,IM)                                 ERAD6950
      GO TO 390                                                         ERAD6960
 1270 IF (CVB.EQ.0.0) GO TO 1290                                        ERAD6970
      DO 1280 I=IN,IM                                                   ERAD6980
 1280 THETA(I) = OLDTH(I)                                               ERAD6990
C                                                                       ERAD7000
C                SET UP FOR ENCALC                                      ERAD7010
C                                                                       ERAD7020
 1290 DO 1300 I=IN,IMP1                                                 ERAD7030
      Q1(I) = 0.                                                        ERAD7040
      RHO(I) = SUMRHO(I)                                                ERAD7050
 1300 X2(I) = SUMX2(I)                                                  ERAD7060
 1310 IF (ZP1(26).EQ.0.0) GO TO 1330                                    ERAD7070
C                                                                       ERAD7080
C                RESTORE NONEQ QUANTITIES                               ERAD7090
C                                                                       ERAD7100
      IF (PUSHA.LT.0.0) GO TO 1320                                      ERAD7110
      CALL NONEQ(IMP1,5)                                                ERAD7120
      GO TO 1330                                                        ERAD7130
 1320 CALL NONEQ(INM1,5)                                                ERAD7140
 1330 RETURN                                                            ERAD7150
      END                                                               ERAD7160
```

REFERENCES

1. Campbell, P. M., and R. G. Nelson, "Numerical Methods for Nonlinear Radiation Transport Calculations," University of California, Lawrence Radiation Laboratory Report, UCRL-7838, September 1964.

2. Kulander, J. L., "Validity of the Eddington Approximation to the Radiative Transport Equation," General Electric Report R65SD14, July 1965.

3. Freeman, B. E., "The Transport Equation for Compton Scattering," General Atomic Informal Report GAMD-6156, March 1965.

4. Freeman, B. E., "The Non-Equilibrium Diffusion Equation," Los Alamos Scientific Laboratory Report LA-3377, September 1965.

5. Triplett, J. R., "SPUTTER, A General Purpose One-dimensional Radiation and Fluid Dynamics Computer Program," General Atomic Report GA-4820, Part I, March 1965.

6. Krook, Max, "On the Solution of Equations of Transfer," Astrophys. J. 122, 488 (1955).

7. Richtmyer, R. D., Difference Methods for Initial-Value Problems, Interscience Publishers, Inc., New York, 1957, p. 102.

8. Ibid, p. 155.

9. Lindley, W. B., "PLNKUT. Evaluation of the Integral of the Planck Function in SPUTTER," General Atomic Informal Report GAMD-6366, May 1965.

10. Barfield, W. D., "A Comparison of Diffusion Theory and Transport Theory Results for the Penetration of Radiation into Plane Semi-infinite Slabs," Los Alamos Scientific Laboratory Report AECD-3653, 1954

11. Richtmyer, R. D., Difference Methods for Initial-Value Problems, Interscience Publishers, Inc., New York, 1964.

12. Cesari, Lamberto, Asymptotic Behavior and Stability Problems in Ordinary Differential Equations, Academic Press, Inc., New York, 1963.

13. Bellman, R., Introduction to Matrix Analysis, McGraw-Hill Book Company, New York, 1960.

SECTION II

SCATTERING METHODS FOR TAMALE

2.1. INTRODUCTION

The TAMALE code (Ref. 1) is a one-dimensional, multifrequency, thermal-radiation, transport code that allows for the finite transit time of photons through the system. (This "retardation" version of the code is currently under development.) This report describes an approach for extending capability of the code to include Thomson scattering, i.e., the scattering of low-energy photons by free electrons.

2.2. ANALYSIS OF THE TRANSPORT EQUATION WITH COMPTON SCATTERING

The calculation of the contribution to radiant energy transfer due to the scattering of photons by free electrons is based on the numerical solution of the relevant radiation transport equation along a selection of sampling rays through the sphere. A discussion of the analysis and logic of the parent code, SPUTTER, is presented in Ref. 2.

The radiation transport equation for the intensity $I(\nu, \vec{\Omega}, r, t)$ with units of energy per unit of frequency, solid angle, time, and area is given by (Ref. 3)

$$\frac{1}{c}\frac{\partial}{\partial t} I(\nu_1, \Omega, r, t) + \Omega_1 \cdot \nabla I(\nu_1, \Omega_1, r, t) = \mu_a (1 - e^{-h\nu_1/\theta}) \Big[B_{\nu_1}(\theta)$$

$$- I(\nu_1, \Omega_1) \Big] - N_e I(\nu_1, \Omega_1) \int d\Omega_2 \frac{d\sigma}{d\Omega_2} \left[1 + \frac{c^2}{2h\nu_2^3} I(\nu_2, \Omega_2) \right]$$

$$+ N_e \left[1 + \frac{c^2}{2h\nu_1^3} I(\nu_1, \Omega_1) \right] \int d\Omega_3 \frac{d\sigma}{d\Omega_1} \frac{\nu_1}{\nu_3} \frac{d\nu_3}{d\nu_1} I(\nu_3, \Omega_3)$$

The first term on the right side represents the quantity of radiant energy absorbed and emitted at frequency ν_1 in direction Ω_1. The second term represents loss of energy by scattering out of the beam Ω_1, ν_1, and the third term the gain by scattering into the beam Ω_1, ν_1. The coefficient N_e is the number of free electrons per unit volume, and μ_a is the absorption coefficient at r for frequency ν_1. The assumptions necessary to derive this equation are as follows:

1. Polarization of photons is neglected.
2. The average kinetic energy of electrons is so small that Doppler effects may be ignored.
3. Local thermodynamic equilibrium (LTE) exists.
4. The electron states are nondegenerate.

Before arriving at an analytical expression for the intensity that is amenable to computer solution, several more assumptions must be made.

The event of a photon being scattered from an electron at rest causes the photon to change frequency. From quantum mechanics one has the Compton formula for the new frequency:

$$\nu_f = \frac{\nu_i}{1 + \gamma_i(1-\mu)}$$

where ν_i, ν_f are the incident and scattered photon frequencies, respectively,

$$\gamma_i = \frac{h\nu_i}{m_o c^2}$$

where m_o is the mass of the electron and c is the speed of light, and $\mu = \Omega_f \cdot \Omega_i$.

A major difficulty in solving the transport equation is that the solid-angle integrations appearing in the scattering terms cannot be performed even if the differential cross sections for scattering, $d\sigma/d\Omega$, are assumed to be simple functions. The reason for this is that the intensity I depends

upon Ω both directly and through the frequency ν, which by the above Compton formula is also a function of Ω through the scattering cosine, μ. To avoid this difficulty, the following assumptions are made:

1. $\gamma < 0.2$
2. $I(\nu_2, \Omega) \approx I(\nu_1, \Omega) + (\frac{\partial I}{\partial \gamma})_1 (\gamma_2 - \gamma_1)$.

The first assumption requires that the photon energies under consideration be small relative to the rest mass of an electron (i.e., $h\nu < 100$ kev). The second assumption requires that the intensity be a smooth function of ν. This approximation is equivalent to the "age" approximation of neutron transport theory. With these approximations the resulting transport equation for Compton scattering in plane or spherically symmetric systems through first order in γ is given by

$$\frac{1}{c}\frac{\partial I}{\partial t} + \vec{\Omega}_1 \cdot \vec{\nabla} I = \mu'_a (B - I) - \mu_s \left\{ I - \frac{3}{16}\int_{-1}^{1} d\mu_3 I(\mu_3)\left[3 - \mu_1^2 + (3\mu_1^2 - 1)\mu_3^2\right] + \gamma \left\{ -2I + \frac{3}{16}\left(1 + \frac{c^2 I}{h\nu_1^3}\right)\int_{-1}^{1} d\mu_3 \left[I - \gamma\left(\frac{\partial I}{\partial \gamma}\right)_3\right] \cdot \left[3 - \mu_1^2 + \mu_1\mu_3(3\mu_1^2 - 5) + (3\mu_1^2 - 1)\mu_3^2 + \mu_1(3 - 5\mu_1^2)\mu_3^3\right]\right\}\right\} + O(\gamma^2)$$

where $\mu_s = (8/3)\pi r_o^2 N_e$ and $\mu'_a = \mu_a(1 - e^{h\nu/\theta})$. Terms of order γ^2 are derived in Ref. 3. The above equation can be further simplified by assuming that stimulated scattering is negligible, i.e., $c^2 I/h\nu_1^3 \ll 1$.

The present development of scattering in TAMALE takes into account only the terms of order zero in γ, which are dominant at low energy, and correspond to restriction of the Compton effect to the limiting case of Thomson scattering. With this approximation, the transport equation for spherical geometry becomes

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mu\frac{\partial I}{\partial r} + \frac{1-\mu^2}{r}\frac{\partial I}{\partial \mu} = \mu'_a(B - I) - \mu_s I + \frac{3}{16}\mu_s\left[(3-\mu^2)\int_{-1}^{1} I(\mu')d\mu'\right.$$

$$\left. + (3\mu^2 - 1)\int_{-1}^{1} I(\mu')\mu'^2 d\mu'\right]$$

Under the transformation

$$x = r\mu \text{ and } y = r\sqrt{1-\mu^2}$$

the above equation reduces to the standard form:

$$\frac{1}{c}\frac{\partial I}{\partial t} + \frac{\partial I}{\partial x} = \mu'_a(B - I) - \mu_s I + \frac{3}{16}\mu_s\left[(3-\mu^2)\int_{-1}^{1} I(\mu')d\mu'\right.$$

$$\left. + (3\mu^2 - 1)\int_{-1}^{1} I(\mu')\mu'^2 d\mu'\right]$$

In the present TAMALE code the capability exists for solving the transport equation with retardation effects but without scattering, or solving the transport equation with scattering but without retardation effects. The treatment of retardation is discussed in Ref. 4 and in Ref. 5 and is not further considered in this report.

With the retardation term $1/c\ \partial I/\partial t$ discarded, the equation to be solved becomes

$$\frac{\partial I}{\partial x} + (\mu'_a + \mu_s)I = \mu'_a B + \frac{3}{16}\mu_s\left[(3-\mu^2)\int_{-1}^{1} I(\mu')d\mu'\right.$$

$$\left. + (3\mu^2 - 1)\int_{-1}^{1} I(\mu')\mu'^2 d\mu'\right] \qquad (38)$$

or

$$I(x_2) = I(x_1)e^{-(\mu'_a + \mu_s)(x_2 - x_1)}$$

$$+ \int_{x_1}^{x_2} \mu'_a B(x')e^{-(\mu'_a + \mu_s)(x_2 - x')} dx' + F_s(x_2) \tag{39}$$

where

$$F_s(x_2) = \frac{3}{16}\mu_s \int_{x_1}^{x_2} \left[(3 - \mu^2) \int_{-1}^{1} I(\mu')d\mu' \right.$$

$$\left. + (3\mu^2 - 1) \int_{-1}^{1} I(\mu')\mu'^2 d\mu' \right] e^{-(\mu'_a + \mu_s)(x_2 - x')} dx'$$

2.3. NUMERICAL SOLUTION OF THE TRANSPORT EQUATION WITH THOMSON SCATTERING

The numerical solution to Eq. (39) above has been developed in Ref. 6. The salient features of this development will be repeated for continuity and ease of reference.

The first two terms on the right side have already been considered in Ref. 2. In evaluating the third term, $F_s(x_2)$, two numerical approximations are made:

1. The radiation energy and pressure vary linearly with x.
2. $\mu^2 \cong x^2/(a^2 + y^2)$, where $a^2 = (x_2 + x_1)^2/4$ and $x_1 \leq x \leq x_2$.

With these assumptions the scattering source contribution can be developed in the following manner:

$$F_s(x_2) = \frac{3}{16}\mu_s \left\{ \left(\frac{1 - e^{\bar{\mu}\Delta}}{\bar{\mu}\Delta}\right) \left[T_o(x_2) + \left(\frac{x_2}{a}\right)^2 T_2(x_2)\right]\Delta \right.$$

$$+\left[\frac{e^{-\bar{\mu}\Delta}(1+\bar{\mu}\Delta)-1}{(\mu\Delta)^2}(T_o(x_2)-T_o(x_1)+\frac{x_2}{a^2}(2T_2(x_2)\Delta+x_2(T_2(x_2)-T_2(x_1))\right]$$

$$+\left(\frac{2-e^{-\bar{\mu}\Delta}[(\mu\Delta)^2+2\bar{\mu}\Delta+2]}{(\bar{\mu}\Delta)^3}\right)(T_2(x_2)\Delta+2x_2(T_2(x_2)-T_2(x_1)))\frac{\Delta^2}{a^2}$$

$$+\left(\frac{e^{\bar{\mu}\Delta}[(\bar{\mu}\Delta)^3+3(\bar{\mu}\Delta)^2+6\bar{\mu}\Delta+6)-6]}{(\bar{\mu}\Delta)^4}\right)(T_2(x_2)-T_2(x_o))\frac{\Delta^3}{a^2} \tag{40}$$

where

$$\Delta = x_2 - x_1$$

$$\bar{\mu} = \mu'_a + \mu_s$$

$$I_k = \int_{-1}^{1} I(\mu)\,\mu^k d\mu$$

$$T_o(x_i) = 3I_o(x_i) - I_2(x_i)$$

$$T_2(x_i) = 3I_2(x_i) - I_o(x_i)$$

To avoid loss of numerical significance when $\bar{\mu}\Delta < 0.1$, the following approximations are used:

$$\left(\frac{1-e^{-\bar{\mu}\Delta}}{\bar{\mu}\Delta}\right) \cong 1 - \frac{\bar{\mu}\Delta}{2}$$

$$\frac{e^{-\bar{\mu}\Delta}(1+\bar{\mu}\Delta)-1}{(\bar{\mu}\Delta)^2} \approx \frac{\bar{\mu}\Delta}{3} - 1/2$$

$$\frac{2-\epsilon^{-\bar{\mu}\Delta}\left[(\Delta\bar{\mu})^2+2\bar{\mu}\Delta+2\right]}{(\bar{\mu}\Delta)^3} \approx 1/3 - \frac{\bar{\mu}\Delta}{4}$$

$$\frac{e^{-\bar{\mu}\Delta}\left[(\bar{\mu}\Delta)^3+3(\bar{\mu}\Delta)^2+6\bar{\mu}\Delta+6\right]-6}{(\bar{\mu}\Delta)^4} \approx \frac{\mu\Delta}{5} - 1/4$$

2.4. THE TAMALE CODE

The coding to incorporate Thomson scattering into TAMALE is contained completely within the subroutines RADTN, TRANS, and RETARD.

The logic of the calculation proceeds exactly as before in the TAMALE code. Three new quantities, μ_s, $T_o(x_i)$, and $T_2(x_i)$ must be available in the RETARD subroutine to complete the calculation. The scattering coefficient μ_s is defined as $K_S\rho$, where K_S is an input number CAPAC(52) and ρ is the material density. In the applications considered, the quantity K_S has been set to .2, corresponding to Z/2 free electrons per atom, where Z is the atomic number. The other two quantities, $T_o(x_i)$ and $T_2(x_i)$, are stored in arrays FI0 (IHNU, x_i) and FI2(IHNU, x_i). These arrays are located in CHUCK common.

An iteration feature has been added to the transport calculation. In solving Eq. (40), the assumption had been made that the intensity $I(x_i, t_n)$ could be evaluated from the moments of the intensity $I_o(x, t_{n-1})$ and $I_2(x, t_{n-1})$ at an earlier time step. This assumption is not valid in general; in particular, on a restart or an initial start the values in the arrays FI0 and F12 are zero, so that there will initially be a decrease in the intensity due to scattering out of the beam but no corresponding increase due to scattering into the beam, and conservation of photons is violated. This problem is alleviated by an implicit iteration procedure. The user has at his disposal two parameters. One parameter is the maximum number of iterations (CAPAC(50)) and the other is the convergence criterion which the functions FI0(IHNU, x_i) and FI2(IHNU, x_i) must satisfy before continuing the calculation (CAPAC(51)).

The input quantities specifically used when Thomson scattering is employed are summarized below (these are also the values used for a sample problem that was solved on the AFWL computer):

Card No.	Quantity	Value	Purpose
77	CVB	1	Specifies all y-lines
2638	CAPAC(50)	10.	Number of iterations
2639	CAPAC(51)	.1	Gives 10% accuracy criterion
2640	CAPAC(52)	.2	Specifies K_S

REFERENCES

1. Spillman, G., "Two Radiation Transport Calculations of Nuclear Weapon Output (HB-1 and HB-2)" (U). Air Force Weapons Laboratory, Report AFWL-TR-66-43, May 1966. (SECRET-RESTRICTED DATA)

2. Freeman, B. E., and C. G. David, "Fireball Phenomenology and Code Development," Vol. III, " SPUTTER Subroutines for Radiation Transport in Spheres," Air Force Weapons Laboratory Report AFWL-TR-65-143, General Atomic Division, General Dynamics Corporation, August 1965.

3. Freeman, B. E., "The Transport Equation for Compton Scattering," General Atomic Informal Report GAMD-6156, March 1965.

4. Freeman, B. E., "Treatment of Retardation in the SPUTTER Radiation Transport Subroutines," General Atomic Informal Report GAMD-5980, December 1964.

5. Palmer, J. T., "A Comparison of Various Difference Schemes for a Simplified One-dimensional Transport Equation," General Atomic Informal Report GAMD-6955, February 1966.

6. Dismukes, C. R., "Treatment of Thomson Scattering of Photons in the SPUTTER Spherical Radiation Transport Subroutines," General Atomic Informal Report GAMD-6536, July 1965.

SECTION III

TWO-DIMENSIONAL RADIATION TRANSPORT TECHNIQUES: A SURVEY OF METHODS

3.1. INTRODUCTION

Several methods for calculating the effects of radiation in hydrodynamical problems have been proposed and tried. In this section, a few of the better methods are compared.

The quantity of interest is the rate of deposition of radiant energy as a function of time and position. The methods to be discussed relate the deposition to the radiant intensity I, which is defined by

$$dE = I(\vec{x}, \vec{\Omega}, \nu, t)\ \vec{\Omega} \cdot d\vec{a}\ d\Omega\ d\nu dt$$

where dE is the amount of radiant energy in a band $d\nu$ of frequencies that flows through an element of area $d\vec{a}$ at $\vec{x}$ in directions contained in the solid angle $d\Omega$ during time interval dt (polarization being neglected). Two related quantities of first importance are the density E and the flux $\vec{F}$ of radiant energy, which are defined as

$$E(\vec{x}, \nu, t) = \frac{1}{c}\int I d\Omega$$

$$\vec{F}(\vec{x}, \nu, t) = \int \vec{\Omega} I d\Omega \qquad (41)$$

The rate of deposition of radiant energy is

$$A = c\int \sigma_d(\vec{x}, \nu, t)\ E\ (\vec{x}, \nu, t) d\nu \qquad (42)$$

where σ_d is a coefficient that depends on the properties of matter at $\vec{x}$, t.

The material will, of course, be radiating energy at some rate $R(\vec{x},t)$, so that the net rate at which it gains energy from the radiation field is A - R.

The equation for transport of radiation is

$$\frac{1}{c}\frac{\partial I}{\partial t} + \vec{\Omega} \cdot \nabla I + \sigma_t I = S \tag{43}$$

where $\sigma_t(\vec{x}, \nu, t)$ is the reciprocal of the mean free path (corrected for induced emission) of photons of frequency ν near $\vec{x}$ at time t, and S is the source, which is defined by

$$dE' = S(\vec{x}, \vec{\Omega}, \nu, t)dVd\Omega d\nu dt$$

where dE' is the amount of radiant energy leaving the element of volume dV around $\vec{x}$ in directions contained in the solid angle $d\Omega$ in the frequency band $d\nu$ during time interval dt. The two contributions to the source are emission

$$S_e(\vec{x},\vec{\Omega},\nu,t) = \frac{\chi(\vec{x},\nu,t)R(\vec{x},t)}{4\pi}$$

where χ is the spectrum, and scattering

$$S_s(\vec{x},\vec{\Omega},\nu,t) = \iint \sigma_s(\vec{x}, \vec{\Omega}' \rightarrow \vec{\Omega}, \nu' \rightarrow \nu, t) \, I(\vec{x}, \vec{\Omega}', \nu', t)d\Omega' d\nu'$$

where σ_s is a coefficient of scattering. Near local thermodynamic equilibrium (LTE),

$$S_e(\vec{x},\vec{\Omega},\nu,t) = \sigma_a(\vec{x}, \nu,t) \, B(\theta(\vec{x},t),\nu)$$

where σ_a is the coefficient of absorption, corrected for induced emission, and B is the Planck function. When departures from LTE are significant, S_e takes a more complicated form, but the problem of how best to calculate it is beyond the scope of this report. The significant point is that S_e is isotropic and strongly temperature dependent.

The methods that are discussed below for finding numerical solutions of the transport equation are of three types: (1) methods that use a finite set of directions, (2) methods that involve the calculation of moments, and (3) Monte Carlo. Methods of the first two types are designed to calculate the intensity I for a given distribution of the source S. But wherever scattering is an important effect, the source depends on the intensity. It then becomes necessary either to iterate to obtain consistency between I and S, or, if sufficiently small time steps are being taken, to use the S from one time step for calculating I at the next time step, or something of this sort. In fact, at frequencies where Compton scattering is important, the calculation of the source may become a major part of the total effort.

In order to keep the discussion as simple and as explicit as possible, only applications using an Eulerian technique to calculate hydrodynamics in an r-z coordinate system (cylindrical coordinates without the angular variable) will be considered. It will further be assumed that the hydrodynamical calculation will advance material properties from time $t = t_{n-1/2}$ to $t = t_{n+1/2}$, assuming that the rates of transfer of radiant energy are held constant at values computed for $t = t_n$. Then radiant intensities and transfer rates are calculated at time t_{n+1}, assuming temperatures, densities, and opacities during the interval $t_n \leq t \leq t_{n+1}$ are as calculated for $t = t_{n+1/2}$.

3.2. THE METHOD OF MOMENTS

The method of moments consists in multiplying the vanishing quantity

$$\mathcal{L} = \frac{1}{c}\frac{\partial I}{\partial t} + \vec{\Omega} \cdot \nabla I + \sigma I - S$$

by each of a set of weighting functions and integrating the products over the domain of $\vec{\Omega}$. Thus,

$$\int 1 \cdot Z d\Omega = \frac{1}{c}\frac{\partial}{\partial t}\int I d\Omega + \nabla \cdot \int \vec{\Omega} I d\Omega + \sigma \int I d\Omega - \int S d\Omega$$

$$= \frac{\partial E}{\partial t} + \nabla \cdot \vec{F} + c\sigma E - \int S d \quad = 0$$

and

$$\int \vec{\Omega} Z d\Omega = \frac{1}{c}\frac{\partial}{\partial t}\int \vec{\Omega} I d\Omega + \nabla \cdot \int \vec{\Omega}\vec{\Omega} I d\Omega + \sigma \int \vec{\Omega} I d\Omega - \int \vec{\Omega} S d\Omega$$

$$= \frac{1}{c}\frac{\partial F}{\partial t} + \nabla \cdot \int \vec{\Omega}\vec{\Omega} I d\vec{\Omega} + \sigma\vec{F} - \int \vec{\Omega} S d\Omega = 0$$

where E and $\vec{F}$ are as defined by Eq. (41). The next step would be to calculate $\int \vec{\Omega}\vec{\Omega} Z d\Omega$, but for present purposes, the calculation will stop with the first moment. It is characteristic of the method that each equation is coupled with the next through the moment of the streaming term $\vec{\Omega} \cdot \nabla I$. Various ways of truncating the system of equations have been proposed. For the purpose of illustration, the simplest of these ways may be chosen, namely, to assume that moments of the intensity beyond a certain order are negligible. Thus, suppose that $I = a_o + \vec{a}_1 \cdot \vec{\Omega}$; in which case

$$E = \frac{1}{c}\int I d\Omega = \frac{4\pi a_o}{c} + \frac{\vec{a}_1}{c} \cdot \int \vec{\Omega} d\Omega = \frac{4\pi a_o}{c}$$

and

$$\vec{F} = \int \vec{\Omega} I d\Omega = a_o \int \vec{\Omega} d\Omega + \vec{a}_1 \cdot \int \vec{\Omega}\vec{\Omega} d\Omega = \frac{4\pi \vec{a}_1}{3}$$

That is,

$$I = \frac{cE + 3\vec{F} \cdot \vec{\Omega}}{4\pi} \tag{44}$$

and

$$\nabla \cdot \int \vec{\Omega}\vec{\Omega} I d\Omega = \nabla \cdot \frac{cE}{4\pi}\int \vec{\Omega}\vec{\Omega} d\Omega + \frac{3}{4\pi}\nabla \cdot \int \vec{\Omega}\vec{\Omega}\vec{\Omega} d\Omega \cdot \vec{F}$$

$$= \frac{c}{3} E\nabla$$

The equations then become

$$\frac{\partial E}{\partial t} + \nabla \cdot \vec{F} + c\sigma E = \int S d\Omega$$

$$\frac{1}{c}\frac{\partial \vec{F}}{\partial t} + \frac{c}{3}\vec{\nabla} E + \sigma \vec{F} = \int \vec{\Omega} S d\Omega \tag{45}$$

This approximation, which is sometimes called non-equilibrium diffusion, has been studied in some detail (see Refs. 1 and 2) and is adequate to describe a wide range of interesting configurations. Nevertheless, formula (44) is not a good representation of radiation which is, say, streaming away from a localized source in a thin medium. Theoretically, the approximation can be improved simply by taking account of more moments. The weighting functions most often used fc. calculating higher moments of functions defined on a sphere are the spherical harmonics, which have the advantage of being orthogonal. However, spherical harmonics are not well adapted to representing the angular dependence of radiant intensity, because the intensity often becomes an almost discontinuous function of angle near abrupt changes in opacity and the expansion of such a function in spherical harmonics converges very slowly. The difficulty cannot, however, be attributed to the use of spherical harmonics. If the intensity were represented as

$$I(\vec{\Omega}) = a_o + \vec{a}_1 \cdot \vec{\Omega} + (\vec{a}_2 \cdot \vec{\Omega})(\vec{b}_2 \cdot \vec{\Omega})$$

$$+ (\vec{a}_3 \cdot \vec{\Omega})(\vec{b}_3 \cdot \vec{\Omega})(\vec{c}_3 \cdot \vec{\Omega}) + \ldots$$

the rate of convergence would be the same. Yvon (see Ref. 3, p.101) has suggested that the convergence could be improved by expanding I_+ and I_- independently, but it is hard to generalize his idea to two dimensions.

Another disadvantage of the method of moments is that the matrix of the finite difference operator yielded by this method as an approximation

to the differential transport operator $(\vec{\Omega} \cdot \nabla + \sigma)$ is rather difficult to invert, so that a time-consuming iterative procedure is required to calculate the intensity at each time step (see, for example, Ref. 4).

3.3. DISCRETE ORDINATES

Wick (Ref. 5), in studying scattering of light in plane atmospheres, got around the difficulty of representing an intensity whose angular distribution is nearly discontinuous by limiting the determination of $I(\vec{\Omega})$ to a fixed finite set of directions $\vec{\Omega}_i$, $i=1,\ldots,n$ which are more or less uniformly distributed. The quantities $I_i = I(\vec{\Omega}_i)$ are the so-called discrete ordinates of the method.

Carlson's S_n method (Ref. 6) is one of the most widely applied numerical versions of the discrete ordinate method. His procedure amounts to replacing the derivatives in the transport equation (43) by finite difference quotients. To do this in finite cylindrical geometry, first set

$$\vec{\Omega} = \mu\vec{k} + (1-\mu^2)^{1/2}(\cos\phi\,\vec{i} + \sin\phi\,\vec{j}) \tag{46}$$

where $\vec{k}$ is a unit vector parallel to the z-axis, $\vec{i}$ is a unit vector perpendicular to $\vec{k}$ and pointing away from the axis of symmetry of the system, and $\vec{j} = \vec{k} \times \vec{i}$. Then $\vec{\Omega} \cdot \nabla I$ can be expressed as a sum of partial derivatives, and the transport equation (43) becomes

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mu\frac{\partial I}{\partial z} + (1-\mu^2)^{1/2}\left(\cos\phi\frac{\partial I}{\partial r} - \frac{\sin\phi}{r}\frac{\partial I}{\partial \phi}\right) + \sigma I = S \tag{47}$$

A discrete system of points in r-z-t space has already been provided by the assumptions concerning the way the hydrodynamics is being computed. It remains only to discretize the angular variables. This is done by selecting a set of μ's that are evenly distributed between -1 and +1. Then ϕ's are chosen for each μ in such a way that the resulting directions are more or less evenly distributed over the unit sphere, for example, as shown in Fig.7.

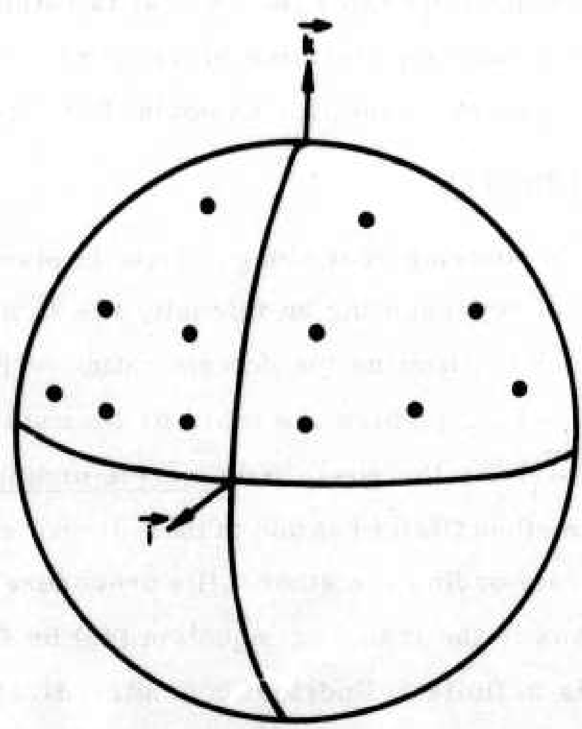

Figure 7. Typical Distribution of Directions.

Having the selected values of ϕ depend on the value of μ causes no difficulty because $\frac{\partial I}{\partial \mu}$ does not occur in the differential equation (47). Let

$$I_{i,\bar{j},\bar{m}} = I(r_i, z_{\bar{j}}, \mu, \phi_{\bar{m}}, \nu, t)$$

where

$$z_{\bar{j}} = 1/2(z_j + z_{j-1}), \quad \phi_{\bar{m}} = 1/2(\phi_m + \phi_{m-1})$$

and μ, ν, and t are fixed. Then it is possible to approximate

$$TI = \mu \frac{\partial I}{\partial z} + (1 - \mu^2)^{1/2} \left(\cos\phi \frac{\partial I}{\partial r} - \frac{\sin\phi}{r} \frac{\partial I}{\partial \phi}\right)$$

by

$$\bar{T}I = 2\mu \frac{I_{\bar{i},\bar{j},\bar{m}} - I_{\bar{i},j,\bar{m}}}{z_j - z_{j-1}} + (1-\mu^2)^{1/2} \left[\cos\phi_{\bar{m}} \frac{I_{i,\bar{j},\bar{m}} - I_{i-1,\bar{j},\bar{m}}}{r_i - r_{i-1}} \right.$$

$$\left. + \frac{2\gamma_m}{r_{\bar{i}}} (I_{\bar{i},\bar{j},\bar{m}} - I_{\bar{i},\bar{j},m-1}) \right]$$

where

$$I_{\bar{i},\bar{j},\bar{m}} = \frac{I_{i,\bar{j},\bar{m}} + I_{i-1,\bar{j},\bar{m}}}{2}$$

$$I_{\bar{i},j,\bar{m}} = 2I_{\bar{i},\bar{j},\bar{m}} - I_{\bar{i},j-1,\bar{m}}$$

$$I_{\bar{i},\bar{j},m} = 2I_{\bar{i},\bar{j},\bar{m}} - I_{\bar{i},\bar{j},m-1}$$

$$\gamma_m = \gamma_{m-1} - \frac{\cos\phi_{\bar{m}} + \cos\phi_{\bar{m}-1}}{2}$$

and

$$\gamma_1 = -\frac{\cos\phi_{\bar{1}}}{2}$$

Here T and $\bar{T}$ denote the differential operator $\vec{\Omega}\cdot\nabla$ and its finite difference approximation, respectively. Then, with the assumption that $I_n = I(r, z, \mu, \phi, \nu, t_n)$, the whole transport equation can be approximated by

$$\frac{1}{c}\frac{I_n - I_{n-1}}{t_n - t_{n-1}} + \frac{\bar{T}I_n + \bar{T}I_{n-1}}{2} + \frac{\sigma_n I_n + \sigma_{n-1} I_{n-1}}{2} = \frac{S_n + S_{n-1}}{2}$$

or

$$\frac{1}{c}\frac{I_n}{t_n - t_{n-1}} + (1/2)(\bar{T}I_n + \sigma_n I_n)$$

$$= \frac{1}{c}\frac{I_{n-1}}{t_n - t_{n-1}} + (1/2)(S_n + S_{n-1} - \bar{T}I_{n-1} - \sigma_{n-1}I_{n-1}) \tag{48}$$

The quantities γ_m, which approximate $\sin \phi_m/\Delta\phi$, are chosen as they are so that the difference equations conserve energy exactly.

A difficulty with the method is that the spatial integration, i.e., the solution of Eq. (48) for some particular value of t, tends to become unstable unless

$$r_i - r_{i-1} < \min \frac{(1 - \mu^2)^{1/2} \cos \phi}{\sigma + \frac{1}{c\Delta t}}$$

at all points, a condition which is very likely to be violated in opaque regions unless the mesh is extraordinarily fine. Various remedies are possible. One is to subdivide the mesh in opaque regions so that the optical distance between neighboring mesh points will be below some limit for all zones in the radiation calculation. Another possibility is to make opaque regions external to the transport calculation since they can be adequately treated in a diffusion approximation anyway. The trouble with the first suggestion is that adding subdivisions to opaque regions can increase the amount of computing that must be done by a sizeable factor. The second suggestion has considerable merit if applied in conjunction with the first, but by itself does not help in regions that are thick enough to be unstable in the S_n method but for which the diffusion approximation is poor.

A possibility that abandons the use of linear difference equations to represent the transport operator is one that Richtmyer (see Ref. 7, p.151) attributes to von Neumann. It is variously called the method of direct

integration or the method of characteristics. The basic idea is the observation that solutions of the transport equation must satisfy the equation

$$I(\vec{x},\vec{\Omega},\nu,t) = I(\vec{x} - s\vec{\Omega},\vec{\Omega},\nu,t - \frac{s}{c})\, e^{-\int_0^s \sigma(\vec{x}-u\vec{\Omega},\nu,t-\frac{u}{c})du}$$

$$+ \int_0^s S(\vec{x} - u\vec{\Omega},\vec{\Omega},\nu,t - \frac{u}{c})\, e^{-\int_0^u \sigma(\vec{x}-v\vec{\Omega},\nu,t - \frac{v}{c})dv}\, du \tag{49}$$

The paths of integration, which are of the form

$$\vec{x} = \vec{x}_o + s\vec{\Omega}$$

$$t = t_o + \frac{s}{c}$$

where the distance s along the path is a parameter, are paths in space-time. They lie on characteristic cones of the differential operator

$$\frac{1}{c}\frac{\partial}{\partial t} + \vec{\Omega} \cdot \nabla$$

which is the basis for the name "method of characteristics." One can use Eq. (49) to estimate the intensity of radiation at some point $\vec{x}$ with coordinates r_i, z_j at some time t_{n+1} and having some direction $\vec{\Omega}_m$ by finding the smallest value of s for which $x - s\vec{\Omega}$ falls on one of the surfaces $r = r_{i\pm 1}$ or $z = z_{j\pm 1}$ or $t = t_n$. Suppose, as shown in Fig. 8, that this point falls on $r = r_{i+1}$ with $z_{j-1} < z < z_j$ and $t_n < t_{n+1} - s/c$. Then, by interpolation, using the points r_{i+1}, z_j and r_{i+1}, z_{j-1} at times t_{n+1} and t_n, one can estimate $I(\vec{x} - s\vec{\Omega}, \vec{\Omega}, \nu, t_{n+1} - \frac{s}{c})$, and then, assuming that one knows σ and S along the path of integration, $I(\vec{x},\vec{\Omega},\nu,t_{n+1})$ can be calculated at $\vec{x} = (r_i, z_j)$. Of

course, some of the required information will be missing unless the calculation proceeds in the proper sequence, e.g., r decreasing and z increasing for $\vec{\Omega}$ pointing somewhat upward and toward the axis. Another point that has been glossed over is the fact that the angle ϕ defined by Eq. (46) changes along the path, so an interpolation involving $\vec{\Omega}$ must also be performed. Interpolation in ϕ is particularly bad and is just what the method of discrete ordinates was supposed to avoid. The S_n method, in which $\partial I/\partial \phi$ is approximated by a difference quotient, suffers from the same malady.

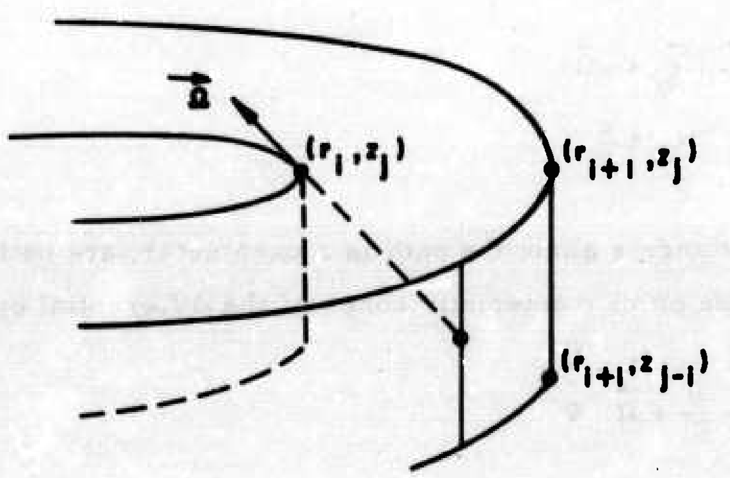

Figure 8. Typical Short Characteristic

The remaining details will not be discussed here; instead the approach will be changed to one avoiding extensive interpolation by integrating Eq. (49) over paths that run straight through the system between pairs of points on the outer boundary. The idea is to ignore the vertices of the mesh and determine the rate of deposition of radiant energy in the zones (which, in the present case, are toroids of rectangular cross section) by suitably averaging the intensities along the paths that they intersect.

The first problem that arises in implementing the method is choosing an appropriate set of paths. The simplest approach is perhaps to choose the paths so that they fill the region of interest more or less uniformly in space and direction. The advantage of this choice is that in calculating rates of deposition of radiant energy from the intensities along the paths, all paths will have about the same weight. To see how lines with the desired uniform distribution can be constructed, define a <u>grid</u> to be a set of parallel lines that intersect a normal plane in a regular pattern of points, e.g., in a square lattice. Next, select a finite set of directions that are more or less uniformly distributed, e.g., the directions from the center of a regular polyhedron to its vertices. Then the set of lines obtained by combining a collection of congruent grids whose directions are those of the selected set will have the desired uniformity. The integration paths are simply obtained as the intersection of the collection of lines with the domain of the hydrodynamical problem, which is a cylinder of finite length.

It is next necessary to consider the problem of calculating intensities and rates of deposition of radiant energy during the time interval $t_n \leq t \leq t_{n+1}$. Suppose that at $t = t_n$ one is given estimates of the intensity at uniformly spaced points along each of the paths. Then, by rewriting (49) as

$$I(\vec{x} + s\vec{\Omega}, \vec{\Omega}, \nu, t + \frac{s}{c}) = I(\vec{x}, \vec{\Omega}, \nu, t)\, e^{-\int_0^s (\vec{x}+u\vec{\Omega}, \nu, t+\frac{u}{c})du} + \int_0^s S(\vec{x} + u\vec{\Omega}, \nu, t + \frac{u}{c})\, e^{-\int_0^u (\vec{x}+v\vec{\Omega}, \nu, t+\frac{v}{c})dv}\, du \tag{50}$$

the intensity can be advanced a distance $c(t_{n+1} - t_n)$ along each path. These pulses of radiation will continually be lost by emerging from the system. They must be replenished by beginning new ones at points where the paths

begin. The initial intensity must be specified as a boundary condition. The energy deposited in a zone during the time interval $t_n \le t \le t_{n+1}$ by radiation of frequency ν may then be estimated to be

$$E = V \frac{\Sigma \int_{s_1}^{s_2} \sigma(\vec{x} + s\vec{\Omega}, \nu, t + \frac{s}{c})\, I(\vec{x} + s\vec{\Omega}, \vec{\Omega}, \nu, t + \frac{s}{c}) ds}{\Sigma (s_2 - s_1)} \tag{51}$$

where the summation is carried out over all paths intersecting the zone, and $s_1 \le s \le s_2$ is the segment of the path that the pulse of radiation, which is located at $\vec{x}$ at time t, sweeps out in the zone during the time interval, and V is the volume of the zone.

The version of the method of characteristics just described has two important advantages: (1) It is possible to traverse optically thick segments in one step, and (2) the three-dimensional interpolation of previously described discrete ordinate methods is avoided.

On the other hand, the method has several disadvantages. One of them is the large number of exponentials that must be calculated. However, this is a reasonable price to pay for being able to traverse long segments, because direct methods for evaluating exponentials are more efficient than finite difference methods, and one can say that, in essence, S_n calculates exponentials by a numerical integration. There are other difficulties connected with the absence of interpolation. For example: (1) the summation in Eq. (51) is a rather crude approximation to an integral over x, $\vec{\Omega}$, and t; (2) if anisotropy of scattering is a significant effect, then the contribution of scattering to the source S in Eq. (50) will be difficult to approximate; (3) in order to get an adequate density of paths near the axis of the system, the density near the boundary must be much higher than necessary; and (4) energy is not conserved in the numerical approximation. Refinements of the method will be left to subsequent reports. It suffices to say that the method can be improved by using some interpolation, but not so much as the earlier versions used.

3.4. THE MONTE CARLO METHOD

The Monte Carlo method discussed below is patterned after one described by Fleck (Ref. 8). As before, the over-all procedure is first to advance the temperature and other material properties from time $t_{n-1/2}$ to time $t_{n+1/2}$ and then to calculate the radiant flux at $t = t_{n+1}$ from that at $t = t_n$, assuming that the average temperature in the time interval $t_n \le t \le t_{n+1}$ is its value at $t = t_{n+1/2}$.

The Monte Carlo procedure involves generating a number of pulses of radiation, called photons, from the given temperature distribution and following them until $t = t_{n+1}$ unless they are absorbed or escape first. Those photons that survive until t_{n+1} are noted, and their histories are continued during the next time interval.

The numerical photons, unlike real ones, all have the same energy E_0. Thus, the number of photons generated in any given zone during the interval $t_n \le t \le t_{n+1}$ is the ratio of the radiant energy liberated by the zone during that interval to the energy E_o of the photons. The fate of a fractional photon is decided by Russian roulette.

The process of following a photon consists first in determining the distance to each of three possible events: (1) penetrating the boundary of a zone, (2) collision, and (3) census. Given the position of a photon and its direction, the distance d_B it has to go before hitting the boundary of the zone it is in can be calculated directly. The distance of the photon from its next collision is

$$d_{col} = -\lambda \log R$$

where λ is the mean distance between collisions, which is a function of the material properties of the zone and the frequency of the photon, and R is a random number drawn from a population distributed uniformly over the real interval $0 \le R \le 1$. The distance to census is simply $d_{cen} = (t_{n+1} - t)/c$.

The event which actually occurs next is the one that occurs within the shortest distance. If it is a collision, a new random number R between 0 and 1 is chosen and compared with the absorption probability p. If $R < p$, the collision is declared to have resulted in an absorption and the history of the photon is terminated. Otherwise, a new direction is chosen according to an appropriate scattering law. If the frequency of the photon is so high that the Compton effect is significant, then the change of frequency must also be calculated.

If the next event is a boundary crossing, either the boundary is an external boundary, in which case the photon is lost, or else it is an interface between zones and the history is continued from the new position and time but without change of direction or frequency. Finally, when a photon reaches census, its state is recorded and its history is continued during the next interval of time.

The amount of energy deposited by the photon as it travels between a pair of consecutive events is estimated to be $E_o \sigma_d s$, where σ_d is the coefficient in Eq. (42), which depends on the frequency of the photon and the state of the zone in which the segment of path lies, and s is the distance between the pair of events. The total amount of radiant energy deposited in each zone during $t_{n-1} \leq t \leq t_n$ is taken to be the sum of such contributions.

3.5. CONCLUSIONS

Among the methods outlined above, Monte Carlo and the method of characteristics appear to be the most promising. The principal advantage of Monte Carlo, in most of its applications, is that it provides a straightforward way to handle the various complications that arise in performing integrations over domains of high dimension. Examples of such complications that occur in problems of radiative transport are retardation, scattering, and, especially in connection with a Lagrangian mesh for describing material properties, geometrical detail. Another advantage of the

Monte Carlo method is that the work can be much reduced if a good estimate of the importance is available. With reference to the present application, this is much the same as saying that the Monte Carlo described above concentrates the numerical work in those regions where the radiant intensity is high because that is where the photons are, whereas the method of characteristics requires about the same amount of calculation in regions of equal size regardless of the intensity.

On the other hand, Monte Carlo methods converge very slowly. Also, while they may provide the best method for obtaining a first estimate of a single multiple integral, they are not generally good for obtaining distributions, which is just what is wanted: the rate of deposition of radiant energy in three dimensions--r, z, and t.

Further, there are two serious disadvantages of the Monte Carlo procedure described above as applied to the particular present problem. One is that the geometrical calculation has to be repeated every time step, whereas in an Eulerian mesh, nonstochastic methods require that geometrical coefficients be calculated only once. The other is that the method will bog down in any hot opaque zone in which a great number of paths will begin and end.

The conclusion is that the method of moments should be used when the first two moments (of degrees 0 and 1) are adequate, and that the method of characteristics should be used when a better transport approximation is required.

REFERENCES

1. Campbell, P., and R. Nelson, "Numerical Methods for Nonlinear Radiation Transport Calculations," University of California, Lawrence Radiation Laboratory Report UCRL-7838, 1964.

2. Freeman, B. E., "The Nonequilibrium Diffusion Equation," Los Alamos Scientific Laboratory Report LA-3377, 1965.

3. Kourganoff, V., Basic Methods in Transfer Problems, Oxford Press, 1952.

4. Gelbard, E., et al., "TRIP-I, A Two-dimensional P_3 Program in X-Y Geometry for the IBM-704," Bettis Atomic Power Laboratory Report WAPD-TM-217, 1960.

5. Wick, G. C., "Ueber Ebene Diffusionsprobleme," Z. Phys. 121 1943.

6. Carlson, B., "Numerical Solution of Neutron Transport Problems." Proceedings of Symposia in Applied Mathematics, Vol. XI, American Mathematical Society, 1961, p. 219.

7. Richtmyer, R. D., Difference Methods for Initial-value Problems, Interscience Publishers, New York, 1957.

8. Fleck, J. A., Jr., "The Calculation of Nonlinear Radiation Transport by a Monte Carlo Method" in Methods in Computational Physics, (B. Alder, S. Fernbach, M. Rotenberg, eds.), Vol. I, Academic Press, New York, 1963, p. 43.

SECTION IV

NON-EQUILIBRIUM DIFFUSION METHODS FOR HECTIC

4.1. INTRODUCTION

The code TDRAD calculates the solution to the two moment equations (45) as the radiation calculation in HECTIC. If we set

$$\int S d\Omega = s \quad \text{and} \quad \int \vec{\Omega} S d\Omega = 0$$

assuming the source to be isotropic, and neglect retardation, the equations become

$$\begin{aligned} &\nabla \cdot \vec{F} + c\,\sigma\, E = s \\ &\frac{c}{3} \nabla E + \frac{\vec{F}}{\lambda} = 0 \end{aligned} \tag{52}$$

Here, $\vec{F}/\lambda$ occurs in place of $\sigma\vec{F}$. An improvement in the approximation can be made by allowing $1/\lambda$ to be unequal to σ because the Planck mean opacity is appropriate for estimating emission and absorption coefficients, while the Rosseland mean is the one to use for transmission coefficients.

In cylindrical coordinates, these equations become

$$\begin{aligned} &\frac{1}{r} \frac{\partial}{\partial r} (r\, F_r) + \frac{\partial}{\partial z} F_z + c\,\sigma E = s \\ &\frac{c}{3} \frac{\partial E}{\partial r} + \frac{1}{\lambda} F_r = 0 \\ &\frac{c}{3} \frac{\partial E}{\partial z} + \frac{1}{\lambda} F_z = 0 \end{aligned} \tag{53}$$

4.2. THE FINITE DIFFERENCE APPROXIMATION

Let r_i, z_j denote the coordinate pair of the mesh point i, j in HECTIC (see Fig. 9). Let $E_{i+1/2,\, j+1/2}$ denote the value of E at the center of

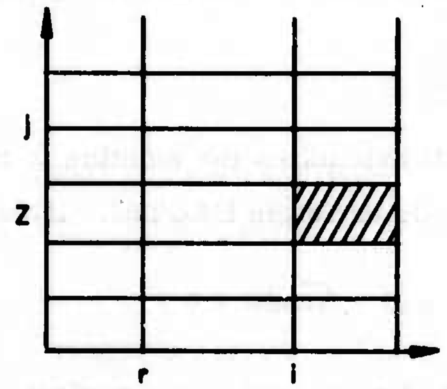

Figure 9. Hydrodynamic Mesh

the zone i, j, i.e., at $r = (r_i + r_{i+1})/2$, $z = (z_j + z_{j+1})/2$. Let $F_{i+1/2,j}$ denote the value F_z at $z = z_j$, $r = (r_i + r_{i+1})/2$, and let $G_{i,j+1/2}$ denote the value of $2\,rF_r$ at $r = r_i$, $z = (z_j + z_{j+1})/2$ (see Fig. 10).

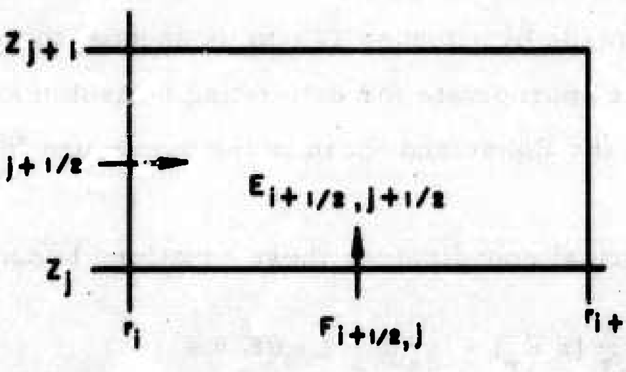

Figure 10. Typical Cell of Mesh

Then a set of difference equations compatible with Eq. (53) is

$$\frac{G_{i+1,j+1/2} - G_{i,j+1/2}}{r_{i+1}^2 - r_i^2} + \frac{F_{i+1/2,j+1} - F_{i+1/2,j}}{z_{j+1} - z_j}$$

$$+ c\sigma_{i+1/2,j+1/2} E_{i+1/2,j+1/2} = s_{i+1/2,j+1/2}$$

$$\frac{2c}{3} \frac{E_{i+1/2,j+1/2} - E_{i+1/2,j-1/2}}{z_{j+1} - z_{j-1}} + \frac{F_{i+1/2,j}}{\lambda_{i+1/2,j}} = 0 \tag{54}$$

$$\frac{4cr_i}{3} \frac{E_{i+1/2,j+1/2} - E_{i-1/2,j+1/2}}{r_{i+1} - r_{i-1}} + \frac{G_{i,j+1/2}}{\lambda_{i,j+1/2}} = 0$$

where

$$\lambda_{i+1/2,j} = \frac{z_{j+1} - z_{j-1}}{\dfrac{z_{j+1} - z_j}{\lambda_{i+1/2,j+1/2}} + \dfrac{z_j - z_{j-1}}{\lambda_{i+1/2,j-1/2}}}$$

$$\lambda_{i,j+1/2} = \frac{r_{i+1} - r_{i-1}}{\dfrac{r_{i+1} - r_i}{\lambda_{i+1/2,j+1/2}} + \dfrac{r_i - r_{i-1}}{\lambda_{i-1/2,j+1/2}}} \tag{55}$$

Eliminating F and G from Eq. (54) gives

$$A_{ij} E_{i-1/2,j+1/2} + B_{ij} E_{i+1/2,j+1/2} + C_{ij} E_{i+3/2,j+1/2}$$
$$+ \alpha_{ij} E_{i+1/2,j-1/2} + \gamma_{ij} E_{i+1/2,j+3/2} + D_{ij} = 0 \tag{56}$$

where

$$A_{ij} = -\frac{4cr_i \lambda_{i,j+1/2}}{3(r_{i+1} - r_{i-1})(r_{i+1}^2 - r_i^2)}$$

$$C_{ij} = -\frac{4cr_{i+1} \lambda_{i+1,j+1/2}}{3(r_{i+2} - r_i)(r_{i+1}^2 - r_i^2)}$$

$$\alpha_{ij} = -\frac{2c\lambda_{i+1/2,j}}{3(z_{j+1} - z_{j-1})(z_{j+1} - z_j)} \tag{57}$$

$$\gamma_{ij} = -\frac{2c\lambda_{i+1/2,j+1}}{3(z_{j+2} - z_j)(z_{j+1} - z_j)}$$

$$B_{ij} = c\sigma_{i+1/2,j+1/2} - A_{ij} - C_{ij} - \alpha_{ij} - \gamma_{ij}$$

$$D_{ij} = -s_{i+1/2,j+1/2} .$$

The boundary conditions are described below. The procedure is to solve Eq. (56) for E, then find F and G using Eq. (54). Finally, the rate at which energy is deposited in the zone i, j is determined by

$$\left(\frac{dE}{dt}\right)_{i+1/2,j+1/2} = \pi\left(z_{j+1} - z_j\right)\left(G_{i,j+1/2} - G_{i+1,j+1/2}\right) + \pi\left(r_{i+1}^2 - r_i^2\right)\left(F_{i+1/2,j} - F_{i+1/2,j+1}\right) \tag{58}$$

4.3. BOUNDARY CONDITIONS

The axis of the system, which corresponds to $i = 0$, is not a geometrical boundary since $r_o = 0$ is required. With reference to Eqs. (56) and (57), $i = 0$ is hardly exceptional since $r_o = 0$ forces $A_{oj} = 0$, which means that $E_{-1/2,j+1/2}$ has a coefficient of 0 and therefore cannot be relevant. Similarly, $G_{o,j+1/2} = 0$, by Eq. (54), which is appropriate for $i = 0$ in Eq. (58).

The outer surfaces can have either blackbody boundary condition or a reflective boundary condition. For a vacuum boundary condition, a blackbody boundary with $\theta = 0$ is used.

The reflective boundary condition is the condition that $\vec{F} \cdot \vec{N} = 0$, where $\vec{N}$ is the normal to the bounding surface. This is equivalent to

$$
\begin{aligned}
G_{I, j+1/2} &= C_{I-1, j} = 0 \quad \text{on the curved boundary} \\
F_{i+1/2, 0} &= \alpha_{i, 0} = 0 \quad \text{on the bottom} \\
F_{i+1/2, J} &= \gamma_{i, J-1} = 0 \quad \text{on the top}
\end{aligned}
\tag{59}
$$

The blackbody boundary condition is analagous to that of ERADTN. (Compare with Eqs. (28) and (29).) Thus,

$$
\begin{aligned}
G_{I, j+1/2} &= 2r_I \, \beta\left(-\frac{ac\,\theta^4}{2} + \frac{c}{2} E_{I-1/2, j+1/2}\right) \\
\frac{1}{\beta} &= 2 - e^{-\alpha(r_I - r_{I-1})/2} \\
\alpha &= \left(\frac{3\mu_{I-1/2, j+1/2}}{\lambda_{I-1/2, j+1/2}}\right)^{1/2}
\end{aligned}
\tag{60}
$$

on the curved boundary $r = r_{I+1}$, $z_j \leq z \leq z_{j+1}$;

$$
\begin{aligned}
F_{i+1/2, o} &= \beta\left(\frac{ac\,\theta^4}{2} - \frac{c}{2} E_{i+1/2, 1/2}\right) \\
\frac{1}{\beta} &= 2 - e^{-\alpha z_1/2} \\
\alpha &= \left(\frac{3\mu_{i+1/2, 1/2}}{\lambda_{i+1/2, 1/2}}\right)^{1/2}
\end{aligned}
\tag{61}
$$

on the bottom; and

$$F_{i+1/2,\,J} = \beta\left(-\frac{ac\theta^4}{2} + \frac{c}{2}E_{i+1/2,\,J-1/2}\right)$$

$$\frac{1}{\beta} = 2 - e^{-\alpha(z_{J+1} - z_J)/2} \tag{62}$$

$$\alpha = \left(\frac{3\mu_{i+1/2,\,J-1/2}}{\lambda_{i+1/2,\,J-1/2}}\right)^{1/2}$$

on the top. Using these formulas in Eq. (54) modifies Eq. (57) at certain points as follows:

on the curved outer surface,

$$C_{I-1,\,j} = 0$$

$$B_{I-1,\,j} = c\,\sigma_{I-1,\,j} + \frac{cr_I\beta}{r_I^2 - r_{I-1}^2} - A_{I-1,\,j} - \alpha_{I-1,\,j} - \gamma_{I-1,\,j}$$

$$D_{I-1,\,j} = -s_{I-1,\,j} - \frac{acr_I\,\beta\theta^4}{r_I^2 - r_{I-1}^2}$$

on the bottom,

$$\alpha_{io} = 0$$

$$B_{io} = c\,\sigma_{io} + \frac{\beta c}{2z_1} - A_{io} - C_{io} - \alpha_{io}, \tag{63}$$

$$D_{io} = -s_{io} - \frac{ac\,\beta\theta^4}{2z_1}$$

on the top,

$$\gamma_{i, J-1} = 0$$

$$B_{i, J-1} = c\,\sigma_{i, J-1} + \frac{\beta c}{2(z_J - z_{J-1})} - A_{I-1, j} - C_{I-1, j} - \alpha_{I-1, j}$$

$$D_{i, J-1} = -s_{i, J-1} - \frac{ac\beta\theta^4}{2(z_j - z_{J-1})}$$

4.4. METHODS FOR SOLVING THE SYSTEM

Sets of equations of the type of Eq. (56) occur widely in the application of finite differences to problems of elliptic partial differential equations. In situations where Eddington's so-called diffusion approximation is good, the splitting method used in MØTET can be used to advantage. However, when Δt is large and the state of the radiation field at time t^{n+1} is essentially decoupled from its state at time t^n, the parabolic character of the problem disappears, and it becomes necessary to turn to methods of the sort used to solve elliptic problems. An iterative method due to Oliphant, which is described briefly in Section 4.5, is used in TDRAD to solve the system (56).

For those problems for which two moments can be expected to provide an adequate description of the field of radiation, Oliphant's method appears to work quite well. When λ becomes large compared with the size of the zones, the method requires an excessive number of iterations to converge. But in these cases, either a full transport approximation is required, or else it is possible to remesh the problem with larger zones.

4.5. PROCEDURE FOR SOLVING THE SYSTEM

Algebraically, the problem of solving the system of equations (56) is that of finding a column vector e that satisfies

$$be = d \tag{64}$$

$$
\begin{aligned}
\text{where } b_{k,k-1} &= A_{ij}, \quad i \neq o \\
b_{k,k} &= B_{ij} \\
b_{k,k+1} &= C_{ij}, \quad i \neq I \\
b_{k,k-I} &= \alpha_{ij}, \quad j \neq o \\
b_{k,k+I} &= \gamma_{ij}, \quad j \neq J \\
e_k &= E_{i+1/2,\, j+1/2} \\
d_k &= -D_{ij} \\
k &= i + jI + 1
\end{aligned}
\tag{65}
$$

The procedure used in TDRAD is due to Oliphant* and is based on the observation that b may be expressed as

$$b = vw + h \tag{66}$$

where $v_{kl} = 0$ unless $k = \ell$, $\ell + 1$, or $\ell + I$; $w_k = o$ unless $k = \ell$, $\ell - 1$, or $\ell - I$; and $h_{k\ell} = 0$ unless $|k - \ell| = I - 1$. The product vw is easy to invert because the factors v and w are triangular. It is plausible to suppose that the iteration

$$e^{(n+1)} = w^{-1} v^{-1} (d - h e^{(n)}) \tag{67}$$

will produce a sequence of approximants $e^{(n)}$ that converge to a solution e of Eq. (64) as $n \to \infty$, and, when b is a matrix arising from a finite difference operator derived from the Laplacian operator, it does, in fact, seem to do so.

Two devices, also recommended by Oliphant, are used to accelerate convergence. The first is to add (K - 1) u to b before performing the

*Oliphant, T. A., "An Extrapolation Procedure for Solving Linear Systems," Quat. Appl. Math. 20, 257 (1962).

factorization (66), u being the part of b above the principal diagonal. To compensate, d is replaced by d + (K - 1) $ue^{(n)}$. The second device is simple extrapolation. Thus,

$$\begin{aligned} e^{(n+1/2)} &= w^{-1}v^{-1}(d + (K-1)\,ue^{(n)} - he^{(n)}) \\ e^{(n+1)} &= \omega e^{(n+1/2)} + (1-\omega)e^{(n)} \end{aligned} \tag{68}$$

The pair of values K,ω has to be determined experimentally. Note that if K = o, the method reduces to a sort of Seidel-method-with-extrapolation, because subtracting u from b leaves it lower triangular and so h = o. Setting K and ω both near 1.0 seems to be close to optimal.

4.6. THE SUBPROGRAM TDRAD

The subprogram TDRAD was designed to carry over essentially all the features of the SPUTTER radiation codes (e.g., multifrequency, opacity tables, time-step controls, boundary conditions) to the HECTIC program with minimum disturbance to the latter, while executing the equations given in Section 4.1. Since the radiation calculation would impose a considerable storage burden, a new COMMON statement with dimensions was worked out for IBM-7044 operation. Cell variables (10 in number for regular HECTIC, with 13 added for radiation) were limited to 400 words each; regular HECTIC provides 1200. All cell variables are assigned storage in a statement COMMON/ARRAY/..

In addition, 29 unsubscripted variables are assigned space in the COMMON block named LINDLY. The names of these variables and brief statements of their significance are given in Table IV. The first 21 variables in LINDLY are the input to TDRAD, and the remaining 8 are computed variables. Table V is a glossary of the variables of greatest importance in TDRAD. A list of some variables, pertinent to the radiation calculation and occurring in TDRAD and HECTIC, for which there exist homologous variables in SPUTTER, is given in Table VI.

Table IV

LINDLY COMMON

Name of Variable	Meaning and/or Function	Value for First Test Problem
SLUG	Arbitrary factor used in time step (accuracy) control pertaining to energy change	0.5
RPTAG	If zero, κ Planck used as is; if nonzero, κ Rosseland used instead	0.0
EFRAC	Constant used to determine importance of energy-poor zones in time step calculation	0.001
DTBUGR	Constant used to change time step as finally calculated	1.0
BCLTAG*	Boundary condition indicator on left or inner radial boundary; inoperative now	0.0
BCRTAG*	Boundary condition indicator on right or outer radial boundary	-1.
BCATAG*	Boundary condition indicator on top axial boundary ("above")	0.
BCBTAG*	Boundary condition indicator on bottom axial boundary ("below")	-1.
MERGE (real)	Multifrequency merge criterion; frequency compared with maximum temperature	0.
CMXK	The K used in adjusting the Oliphant iterative matrix inversion	1.4
CMXOM	The ω used in adjusting the Oliphant iterative matrix inversion	1.0
ERRCRT	Convergence error criterion on matrix inversion iteration	0.001
DBGPRT	Nonzero provides debug print	1.0
DIANTP	Logical tape unit on which DIANE tape is to be hung if one is used	0.0

*In all cases, negative = reflection; zero is vacuum; positive is blackbody whose temperature is value of indicator.

Table IV (continued)

Name of Variable	Meaning and/or Function	Value for First Test Problem
DGREY	If nonzero, DIANE tape is used for a grey calculation	0.0
CAPIN	Value of absorption coefficient assumed if no DIANE tape is read	1.0
ODDC	Optical depth difference criterion; average optical depth not calculated if zone depths are too dissimilar	0.333
MFTAG	If nonzero, multifrequency calculation; otherwise, grey calculation	0
IMPTAG	If nonzero, fully implicit calculation is done; inoperative at present	0
ITAG	Indicator of whether or not to iterate on time-centered temperature; nonzero says "do iterate"	0
ITRMAX	Maximum allowed number of iterations in the matrix inversion	30
	(Computed Variables, i.e., not input)	
SGNL	Material counter for multi-DIANE-tape problems; used in KAPPA and DIANA	
IHNU	Frequency index	
NHNU	Total number of frequency bands	
HNUP	Frequency at upper end of band	
NT	DIANE tape unit	
DHNU	Width of frequency band	
THICK	Not used	
NY	Temperature iteration index	

Table V

PARTIAL GLOSSARY OF FORTRAN VARIABLES

FORTRAN Variable Name	Designation in Difference Equations	Comments
ALAMH (K)	$\lambda_{i+1/2, j}$	K = i + j I + 2
ALAMV (K)	$\lambda_{i, j+1/2}$	
DY (J)	$z_{j+1} - z_j$	
ROSS (K)	$1/\lambda_{i+1/2, j+1/2}$	Rosseland mean opacity, in cm^{-1}
DTAUR	$\frac{r_{i+1} - r_i}{\lambda_{i+1/2, j+1/2}}$	
DTAUL	$\frac{r_i - r_{i-1}}{\lambda_{i-1/2, j+1/2}}$	
DTAUA	$\frac{z_{j+1} - z_j}{\lambda_{i+1/2, j+1/2}}$	
DTAUB	$\frac{z_j - z_{j-1}}{\lambda_{i+1/2, j-1/2}}$	
PUR (I)	$\frac{1}{r_{i+1}^2 - r_i^2}$	defined in the loop DO 150
RUR (I)	$\frac{4}{3} c \frac{\gamma i}{r_{i+1} - r_{i-1}}$	
PUZ (J)	$\frac{1}{z_{j+1} - z_j}$	defined in the loop DO160
RUZ (J)	$\frac{2}{3} c \frac{1}{z_{i+1} - z_{j-1}}$	
X(I)	r_{i+1}	Note displacement of index
Y(J)	j+1	Note displacement of index

Table V (continued)

FORTRAN Variable Name	Designation in Difference Equations	Comments
XA(K)	A_{ij}	Defined two lines above statement 531
XC(K)	C_{ij}	Defined at statement 536
XALP(K)	α_{ij}	Defined one line below statement 540
XGAM(K)	γ_{ij}	Defined at statement 546
XD(K)	$-D_{ij}$	
XB(K)	B_{ij}	
PLANCK (K)	$\sigma_{i+1/2, j+1/2}$	Planck mean opacity, in cm^{-1}
B (K)	κ	Source; not explicitly referred to in text
XD (K)	$E_{i+1/2, j+1/2}$	Radiation energy, redefined in matrix inversion
XA (K)	$F_{i+1/2, j}$	Flux; redefined two lines above statement 650
XB (K)	$G_{i, j+1/2}$	Flux; redefined one line below statement 655

Table VI

BERLITZ GUIDE TO TDRAD FOR THE SPUTTER USER

Name of HECTIC or TDRAD Variable	Name of Sputter Variable
MFTAG	KMAX
RPTAG	SOLID (10)
EFRAC	TELM (37)
IMPTAG	HVB
DTBUGR	TELM (25)
NRM = Z (62)	NTIMES = BOILB
NR	NRAD
DT = Z (3)	DTH2
BCLTAG	GA
BCRTAG	GL
BCBTAG	
BCATAG	
MERGE	CB
ROSS	CAPAR
PLANCK	CAPAC
B	X6
ØDDC	AC (ERADTN only)
DBGPRT	S12
DIANTP	AMASNO(L+17)
DGREY	S15

4.7. OUTLINE OF TDRAD

1. Set up temperature iteration index and turn off divide check light.
2. Call KAPPA and thereby obtain the grey opacities, expressly for the time step calculation.
3. Calculate time step for each zone by two criteria, stability and (energy) accuracy.
4. Find minimum time step and set subcycle quantities if necessary.
5. Test divide check light, calculate geometry factors (saves time but costs storage to do this at this early part of the code), and find the largest temperature. The largest temperature is used only in deciding whether or not to merge frequency groups in a multifrequency calculation. Zero several zone quantities.
6. If doing multifrequency calculation, and if there are frequency groups with too large $u = h\nu/\theta$, merge them together.
7. If doing grey calculation, evaluate source B, set extreme frequency limits, and transfer to (9).
8. If doing a normal multifrequency calculation, update frequency parameters and evaluate source, B.
9. Set blackbody sources if appropriate and test divide check light.
10. Form zone and edge $\kappa\rho$.
11. Form and modify matrix elements.
12. Invert matrix iteratively.
13. Calculate radiation flux and internal energy change.
14. End frequency loop.
15. Iterate on temperature.
16. Reset temperature if necessary and return.

4.8. REVIEW OF THE CODE DEVELOPMENT

In early January 1966 the iterative version was written, and test problems were begun. A rather "thick" problem (one mean free path per cell) was tried, and the results appeared satisfactory after a brief debug phase. Then a run was made to compare directly with ERADTN, with a reflective

outer radial boundary condition chosen to simulate a problem in slab geometry. The interior of this slab comparison was quite thin, and convergence difficulties arose. It was found, after several trials, that a choice of parameters K = 1.2, ω = 1.0 (see Section 4.6) was best for this particular problem. Other problems to test the effects of non-squareness of logical mesh (the test problem was 5 x 50) and thinness were run. It was found that both factors contribute to slow convergence. In February 1966, considerable effort was expended on a different test problem, a thin hot sphere radiating into a thinner, cold medium. The following initial conditions were used:

$\theta = 5.081 \times 10^{-1}$ ev

$\rho_o = 5.29 \times 10^{-2}$ g with ambient density $\rho_A = 1.89 \times 10^{-4}$

HVB = 4.2×10^{16} erg

HCB = 1.3×10^{10} erg

CV = 2.6×10^{10} erg

HCP = $4. \times 10^{9}$ erg

I = 5.5×10^{10} erg, of which only 4.0×10^{9} erg is allowed to gc into vapor

$\gamma = 1.5$

A perfect gas equation of state was used to describe the vapor expansion. The radiation boundary conditions used are shown in Fig. 11.

A study was made of the convergence of the radiation equation. Various values of K and ω which are used to adjust the iterative matrix inversion were tried. As a result of these tests, the following observations were made:

1. If $E_{i+1/2, j+1/2}$ goes negative for any reason, even if it is subsequently set to zero, the convergence criterion is very hard to meet.

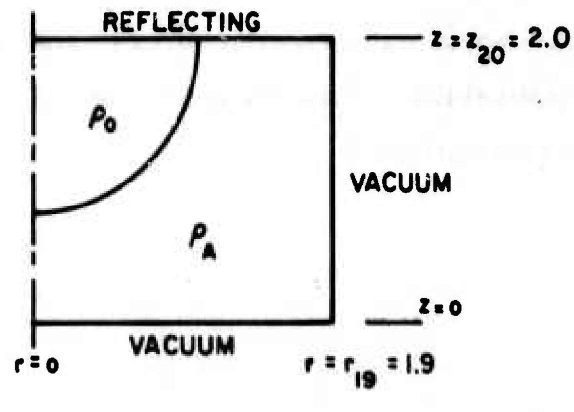

Figure 11. Configuration of Test Problem

2. For $E_{i+1/2, j+1/2}$ always greater than zero, the following seems to be true:

   a. Initial $E = 137\ \theta^4$ seems to converge over the entire mesh faster than $E = 0$.

   b. $|\Delta E|_i$ for cells with max E is generally only slightly larger than $|\Delta E_i|$ for cell with min E.

In April, a subroutine for completely factoring b was written. Thus,

$$b = vw$$

where $v_{ij} = o$ unless $j \leq i \leq j + I$ and $w_{ij} = o$ unless $j - I \leq i \leq j$. Although this closed method is inferior to the iterative method in all respects — space and time consumed and accuracy — it is a useful diagnostic tool for small test problems because it eliminates the question of convergence. The technique was accommodated by writing all 22 cell arrays on a tape and using the corresponding storage to invert the matrix, limiting I (say, the number of radial columns of cells in a HECTIC mesh) to 22. This version was written and executed, with reasonably satisfactory results. The thin sphere, described above, was tried, and the resulting radiation energy distribution looked about right. However, the radiant flux gradient, which determines actual energy transfer, was quite small and noisy. The

question of limitations on numerical accuracy, and the related question of the range of applicability of the diffusion method to optically thin media, are both under investigation.

4.9. APPENDIX: LISTING OF TDRAD

```
$IBFTC TDRAD   LIST,DECK,REF
      SUBROUTINE  TDRAD
COMPILED JANUARY 27, 1966     WBL
C
C                 D   I   M   E   N   S   I   O   N
C
                           DIMENSION
     1U( 400),       V( 400),       AMX( 400),     AIX( 400),     P( 400),
     2THETA( 400), RHO( 400),     FIOUT( 400), CAP( 400),      KFIT( 400),
     3            IW1(50),W2(50),W3(50),TABLM(50),
     4DX(52),       X(53),         XX(54),        DY(100),       Y(100),       YY(101),
     5TAB(15),      AMK(15),       PK(15),        QK(15),        Z(150),       IZ(150),
     6TAU(52),      PL(200),       PR(200),       UL(200),       UR(200),
     7FLEFT(100),YAMC(100),SIGC(100),GAMC(100),
     8G(50),SOLID(400),TEMP(12)
      COMMON           Z        ,XX      ,UR      ,PR      ,THETA   ,YY
      COMMON           AID      ,AIX     ,AM      ,AMD     ,AMX     ,AREA
      COMMON           BIG      ,BOUNCE  ,DDXN    ,DDVK    ,DVK     ,DX
      COMMON           DY       ,E       ,FD      ,FS      ,FX      ,OUT
      COMMON           P        ,PABOVE  ,PBLO    ,PIDTS   ,PPABOV  ,PRR
      COMMON           PUL      ,QDT     ,RC      ,REZ     ,RHO     ,RL
      COMMON           RR,SIG,Q000FL,SWITCH ,TABLM,TAU
      COMMON           TAUDTS   ,TAUDTX  ,U       ,UK      ,URR     ,UT
      COMMON           UU       ,UUU     ,UTEF    ,UVMAX   ,V       ,VABOVE
      COMMON           VBLO     ,VEL     ,VK      ,VT      ,VTEF    ,VV
      COMMON           VVABOV   ,VVBLO   ,W2      ,W3      ,WPS     ,WS
      COMMON           WSA      ,WSB     ,WSC     ,XL      ,XLF     ,XN
      COMMON           XR       ,YL      ,YLW     ,YN      ,YU      ,ZMAX
      COMMON           I        ,II      ,IN      ,IR      ,IWS     ,IWSA
      COMMON           IWSB     ,IWSC    ,IW1     ,J       ,JN      ,JP
      COMMON           JR       ,K       ,KN      ,KP      ,KR      ,KRM
      COMMON           L        ,M       ,MA      ,MB      ,MC      ,MD
      COMMON           ME       ,MZ      ,N       ,NK      ,NKMAX   ,NK1
      COMMON           NO       ,NR      ,G       ,SOLID   ,TEMP
      COMMON           FIOUT    ,CAP     ,KFIT
C
C
C
C              E   Q   U   I   V   A   L   E   N   C   E
     0EQUIVALENCE      (Z,IZ,PROB),       (Z(2),CYCLE),       (Z(3),DT),
     1(Z(4),PRINTS),   (Z(5),PRINTL),     (Z(6),DUMPT7),      (Z(7),CSTOP),
     2(Z(8),PIDY),     (Z(9),TMZ),        (Z(10),GAM),        (Z(11),GAMD),
     3(Z(12),GAMX),    (Z(13),ETH),       (Z(14),FFA),        (Z(15),FFB),
     4(Z(16),TMDZ),    (Z(17),TMXZ),      (Z(18),XMAX),       (Z(19),TXMAX),
     5(Z(20),TYMAX),   (Z(21),AMDM),      (Z(22),AMXM),       (Z(23),DNN),
     6(Z(24),DMIN),    (Z(25),FEF),       (Z(26),DTNA),       (Z(27),CVIS),
     7(Z(28),NPR),     (Z(29),NPRI),      (Z(30),NC),         (Z(31),NPC),
     8(Z(32),NRC),     (Z(33),IMAX),      (Z(34),IMAXA),      (Z(35),JMAX),
     9(Z(36),JMAXA),   (Z(37),KMAX),      (Z(38),KMAXA),      (Z(39),NMAX)
     0EQUIVALENCE      (Z(40),ND),        (Z(41),KDT),        (Z(42),IXMAX),
     1(Z(43),NOD),     (Z(44),NOPR),      (Z(45),NIMAX),      (Z(46),NJMAX),
     2(Z(47),I1),      (Z(48),I2),        (Z(49),I3),         (Z(50),I4),
     3(Z(51),N1),      (Z(52),N2),        (Z(53),N3),         (Z(54),N4),
     4(Z(55),N5),      (Z(56),N6),        (Z(57),N7),         (Z(58),N8),
     5(Z(59),N9),      (Z(60),N10),       (Z(61),N11),        (Z(62),NRM),
     6(Z(63),TRAD),    (Z(64),XNRG),      (Z(65),SN),         (Z(66),DXN),
     7(Z(67),RADER),   (Z(68),RADET),     (Z(69),RADEB),      (Z(70),DTRAD),
     8(Z(71),REZFCT),  (Z(72),RSTOP),     (Z(73),SHELL),      (Z(74),BBOUND),
     9(Z(75),TOZONE),  (Z(76),ECK),       (Z(77),SBOUND),     (Z(78),X1)
     0EQUIVALENCE      (Z(79),X2),        (Z(80),Y1),         (Z(81),Y2),
     1(Z(82),CABLN),   (Z(83),VISC),      (Z(84),T),          (Z(85),GMAX),
     2(Z(86),WSGD),    (Z(87),WSGX),      (Z(88),GMADR),      (Z(89),GMAXR),
     3(Z(90),S1),      (Z(91),S2),        (Z(92),S3),         (Z(93),S4),
     4(Z(94),S5),      (Z(95),S6),        (Z(96),S7),         (Z(97),S8),
     5(Z(98),S9),      (Z(99),S10)
C
```

```
      0EQUIVALENCE      (Z(100),HVB),     (Z(101),HCB),     (Z(102),CB),
      1(Z(103),SVS),    (Z(104),ATOM),    (Z(105),CV),      (Z(106),GV),
      2(Z(107),SUMFE),  (Z(108),BETA),    (Z(109),ALCO),    (Z(110),ANN),
      3(Z(111),EZERO),  (Z(112),PW),      (Z(113),CAPS),    (Z(114),HNU),
      3(Z(115),COE),    (Z(116),SCR),     (Z(117),ISR),     (Z(118),SCDR),
      4(Z(119),AHN),    (Z(120),DTH),     (Z(121),IH),      (Z(122),JH),
      5(Z(123),DTC),    (Z(124),IC),      (Z(125),JC),      (Z(126),RFT),
      X(Z(127),CDUT),   (Z(128),HCP),     (Z(129),HH),      (Z(130),CO),
      6(Z(131),J1),     (Z(132),J2),      (Z(133),J3),      (Z(134),J4),
      7(Z(135),J5),     (Z(136),J6)
      0EQUIVALENCE      (Z(140),VAPE),    (Z(141),RADE),    (Z(142),CNDE),
      1(Z(143),SCRE)
C
      0EQUIVALENCE      (XX(2),X(1)),     (UR,UL,FLEFT),    (UR(100),YAMC),
      1(PR(100),SIGC),  (PR,PL,GAMC),     (DKE,THETA),      (UR,TAB),
      2(UR(16),AMK),    (UR(31),PK),      (UR(46),QK),      (YY(2),Y(1))
C
C
       COMMON  /LINDLY/  SGNL, IHNU, NHNU, HNUP, N., DHNU, THICK, NY,
      2 MFTAG, SLUG, RPTAG, EFRAC, IMPTAG, DTBUGR, BCLTAG, BCRTAG, ITAG,
      3 BCBTAG, BCATAG, MERGE, CMXK, CMXOM, ERRCRT, ITRMAX, DRGPRT,
      4 DIANTP, DGREY, CAPIN, ODDC
       COMMON  /ARRAY/  ROSS( 400), PLANCK( 400), ER( 400), XCV( 400),
      2 XA( 400), XB( 400), XC( 400), XALP( 400), XGAM( 400), B( 400),
      3 XD( 400), ALAMH( 400), ALAMV( 400), XG( 400), ERAD( 400),
      4 OLDTH( 400)
C                 C        O        M        M        O        N
       DIMENSION  PUR(50), PUZ(100), RUR(50), RUZ(100), BETAB(50),
      2 BETAA(50), BETAR(100)
       REAL  MERGE
    4 FORMAT  (7H1CYCLE F6.0, 7H  TIME 1PE13.6, 5H  DT 1PE13.6/)
    5 FORMAT  (                   4X1HK, 11X2HXA, 11X2HXB, 11X2HXC, 11X2HXD
     2, 9X4HXALP, 9X4HXGAM, 12X1HB, 9X4HROSS, 7X6HPLANCK/)
    6 FORMAT  (I5,  1P9E13.6)
    7 FORMAT  (1H13X1HK, 7X6HV FLUX, 7X6HH FLUX, 6X7HDELTA E)
    8 FORMAT  (/10H ITERATIONI4, 22H  MAX. RELATIVE ERROR 1PE9.3,
     2 7H  ZONE I4, 14H  ZONE ENERGY 1PE9.3)
    9 FORMAT  (3H XG)
   10 FORMAT  (5H ERAD)
   11 FORMAT  (1P10E12.5)
C     NY(IN LINDLEY COMMON) IS TEMPERATURE ITERATION INDEX USED IN KAPPA.
      IF (MFTAG .EQ. 0)  DHNU = 1.
      NVEZ = 1                                                          DRAD 101
      NY = NVEZ                                                         DRAD 104
      IF (ITAG .EQ. 0)  NVEZ = 2
      VEZ = NVEZ                                                        DRAD 103
      CALL DVCHK (KDMY)
C                                                                       DRAD 106
C           FORM MONOFREQUENCY QUANTITIES AND FIND MIN TIME STEP        DRAD 107
C                                                                       DRAD 108
      WSB = 0.0                                                         DRAD 109
      DO  1076  K = 2, KMAX
 1076 WSB = WSB + AIX(K) * AMX(K)
      DTR1=1.E10                                                        DRAD 112
      DTR2=1.E10                                                        DRAD 113
      IHNU = 0                                                          DRAD 119
      CALL KAPPA
C     MUST FORM LOG OF TEMPERATURE AND DENSITY IN KAPPA
 1080 DO  1230  I = 1, IMAX
      K = I + 1
      DO  1229  J = 1, JMAX
CALL UNCLE IF EITHER KAPPA IS ZERO OR NEGATIVE                          DRAD 122
      IF (AMIN1(PLANCK(K), ROSS(K)) .GT. 0.0)  GO TO 1120
      S1=13.1090                                                        DRAD 124
      CALL UNCLE                                                        DRAD 125
```

```
 1120 TEMP(1)=SQRT(PLANCK(K) * ROSS(K))
      TEMP(3) = PLANCK(K)
      IF  (RPTAG .EQ. 0.0) GO TO 1125
      TEMP(1) = ROSS(K)
      TEMP(3) = ROSS(K)
 1125 IF(0.001 - THETA(K)) 1160,1230,1230
 1160 DELTAU = 0.5 * TEMP(1) * RHO(K)
      TEMP(1) = 1.E10                                                   DRAD 131
      TEMP(2) = 1.E10                                                   DRAD 132
      IF (ER(K).EQ.0.) GO TO 1170
      WSBB = AIX(K) * AMX(K)
      IF (EFRAC    .EQ. 0.0)  GO TO 1170
      IF (WSBB - EFRAC    * WSB)  1170, 1165, 1165
C     ACCURACY CRITERION -- DONE UNCONDITIONALLY                        DRAD 137
 1165 TEMP(1) = SLUG * AMX(K) / ABS(ER(K)) * AIX(K)
 1170 IF (MFTAG .EQ. 0    .AND. IMPTAG .NE. 0  )  CONTINUE
C     GO TO 1172 REPLACED BY CONTINUE UNTIL FULLY IMPLICIT CODING IS PUT IN
C     STABILITY CRITERION -- BYPASSED IN FULLY IMPLICIT CASE            DRAD 140
      DENOM = 4.1132E12 * TEMP(3) * THETA(K)**4 / AIX(K)
      TEMP(2) = (0.5 + 1.5 * (DELTAU * AMIN1(DX(I), DY(J)))**2) / DENOM
 1172 TEMP(2) = AMIN1(TEMP(1), TEMP(2))                                 DRAD 142
      TEMP(2)=TEMP(2)*DTBUGR
C***********************************************************************DRAD 144
C                                                                      *DRAD 145
C              F I N D   M I N I M U M   T I M E   S T E P             *DRAD 146
C                                                                      *DRAD 147
C***********************************************************************DRAD 148
      IF (TEMP(2)) 1230,1230,1190                                       DRAD 149
 1190 IF (TEMP(2)-DTR1) 1200,1210,1210                                  DRAD 150
 1200 DTR2=DTR1                                                         DRAD 151
      KMN2=KMN1
      DTR1=TEMP(2)                                                      DRAD 153
      KMN1=K
      GO TO 1230                                                        DRAD 155
 1210 IF (TEMP(2)-DTR2) 1220,1230,1230                                  DRAD 156
 1220 DTR2=TEMP(2)                                                      DRAD 157
      KMN2=K
 1229 K = K + IMAX
 1230 CONTINUE                                                          DRAD 159
      DTRMIN=DTR1                                                       DRAD 160
C                                                                       DRAD 162
C              PRINT MINIMUM TIME STEPS BETWEEN EDITS                   DRAD 163
C              DELETED UNTIL WE KNOW THE OIL PRINT ROUTINE
C                                                                       DRAD 172
C         DETERMINE IF RADIATION OR HYDRO WILL SUBCYCLE                 DRAD 173
C              NO HYDRO SUBCYCLE IN THIS VERSION                        DRAD 174
C     FOR INITIAL START, DT AND TRAD NEED TO BE PROVIDED AS INPUT.
CAVEAT.  OIL PROBABLY DOES THINGS DIFFERENTLY.
      IF (DTRMIN - TRAD)  1280, 125, 125
C***********************************************************************DRAD 180
C                                                                      *DRAD 181
C                  R E D U C E   T I M E   S T E P                     *DRAD 182
C                                                                      *DRAD 183
C***********************************************************************DRAD 184
 1280 NR = DT / DTRMIN + 1.0
      TRAD = DT / FLOAT(NR)
      IF (NR .LE.     NRM )   GO TO 125
 1290 S1=13.1290                                                        DRAD 188
      CALL UNCLE                                                        DRAD 189
  125 THTAMX=.025                                                       DRAD 195
      CALL DVCHK(KDMY)
      GO TO (127, 130), KDMY
  127 S1 = 13.0127
      CALL UNCLE
C     CALCULATE GEOMETRY FACTORS AND FIND HIGHEST TEMPERATURE           DRAD 197
```

```
  130 DO  150  I = 1, IMAX
      PUR(I  ) = PIDY / TAU(I  )
  150 RUR(I+1) = 4.0E10 * X(I) / (X(I+1) - X(I-1))
      DO  160  J = 1, JMAX
      PUZ(J  ) = 1. / DY(J  )
  160 RUZ(J+1) = 2.0E10 / (Y(J+1) - Y(J-1))
      DO  180  K = 2, KMAX
      IF (THETA(K) .LE. THTAMX)  GO TO 180
      THTAMX=THETA(K)
  180 CONTINUE
      THTAMX = AMAX1(THTAMX, BCLTAG, BCRTAG, BCBTAG, BCATAG)                DRAD 211
C     REENTRY POINT FOR SECOND TEMPERATURE ITERATION
  200 DO 210 K = 2, KMAX
      XA(K) = 0.
      XB(K) = 0.
      XC(K) = 0.
      XALP(K) = 0.
      ER(K) = 0.0
  210 XGAM(K) = 0.
C
C                                                                          DRAD 242
C************************************************************************ DRAD 243
C                                                                         *DRAD 244
C                 B E G I N   F R E Q U E N C Y   L O O P                 *DRAD 245
C                                                                         *DRAD 246
C                                                                         *DRAD 247
C*************************************************************************DRAD 248
C                                                                          DRAD 249
C               SET UP MAX FREQ BOUNDARY                                   DRAD 250
C                                                                          DRAD 251
      HNUP=1.0E6
      HNUP4=1.0E24
      IF (MFTAG .EQ. 0)    GO TO 280
  220 IHNU = IHNU + 1
      CALL KAPPA
      HNU4=HNU**4
      DHNU = HNUP - HNU                                                    DRAD 258
C                                                                          DRAD 260
C     MERGE GROUPS WITH HNU MORE THAN (MERGE) TIMES LARGEST THETA          DRAD 261
C
      IF (MERGE  .GT. 0.0)  GO TO 225                                      DRAD 263
      SI = 13.0225
      CALL UNCLE                                                           DRAD 265
  225 IF  (THTAMX - HNU / MERGE)  240, 230, 230                            DRAD 266
  230 IF (IHNU - 1)  235, 370, 260
  235 SI = 13.0235                                                         DRAD 268
      CALL UNCLE                                                           DRAD 269
C                                                                          DRAD 270
C              REJECT TAPE IF MORE THAN HALF OF GROUPS MERGE               DRAD 271
C                                                                          DRAD 272
  240 IF (IHNU+IHNU-NHNU) 260,250,250                                      DRAD 273
  250 IF (AMOD(MERGE,1.) .EQ. 0.5)  GO TO 260                              DRAD 274
      SI=13.0250
      CALL UNCLE                                                           DRAD 276
  260 DO 270 K = 2, KMAX                                                   DRAD 277
      T4 = THETA(K)**4
      BETA=HNU/THETA(K)
      BETAP=HNUP/THETA(K)
      DFB=PLNKUT(BETA,BETAP)
      IF (DFB.EQ.0.) GO TO 270                                             DRAD 281
      TEMP(1) = DFB * T4                                                   DRAD 282
      EMB1=EXP(-BETA)
      EMB2=EXP(-BETAP)                                                     DRAD 284
      TEMP(2)=DFB+0.0384974 / T4 *(HNU4/(1.0-EMB1)                         DRAD 285
     1*EMB1-HNUP4/(1.0-EMB2)*EMB2)
C                                                                          DRAD 287
                                                                           DRAD 288
```

```
C                 FORM NUMERATORS AND DENOMINATORS OF MERGED KAPPAS            DRAD 289
C                                                                              DRAD 290
      XA(K)=XA(K)+TEMP(1)
      XB(K)=XB(K)+TEMP(2)
      XC(K) = XC(K) + PLANCK(K) * TEMP(1)
      XALP(K) = XALP(K) + TEMP(2) / ROSS(K)
  270 CONTINUE                                                                 DRAD 295
      HNUP=HNU                                                                 DRAD 296
      HNUP4=HNU4                                                               DRAD 298
      IF (THTAMX- HNU/ MERGE) 220,310,310
C                                                                              DRAD 300
C                 FORM MERGED KAPPAS                                           DRAD 301
C                                                                              DRAD 302
  310 DO 350 K = 2, KMAX
      IF (XA(K)) 320,350,330
  320 S1=13.0320                                                               DRAD 305
      CALL UNCLE                                                               DRAD 306
  330 ROSS(K) = XB(K) / XALP(K)
      PLANCK(K) = XC(K) / XA(K)
  350 CONTINUE                                                                 DRAD 309
      HNUP=1.0E6
      HNUP4=1.0E24
      DHNU = HNUP - HNU                                                        DRAD 312
      GO TO 480
C                                                                              DRAD 315
C                 MONOFREQUENCY CALCULATION                                    DRAD 316
C                                                                              DRAD 317
  280 NHNU=1                                                                   DRAD 318
       IHNU = 1
      DO 290 K = 2, KMAX
  290 B(K) = THETA(K)**4
      HNU = .001                                                               DRAD 326
      GO TO 480                                                                DRAD 327
C                                                                              DRAD 328
C                 TYPICAL GROUP CALCULATION OF SOURCES                         DRAD 329
C                                                                              DRAD 330
  360 IHNU = IHNU +1
      CALL KAPPA
      DHNU=HNUP-HNU                                                            DRAD 332
      HNU4=HNU**4                                                              DRAD 333
  370 DO  392  K = 2, KMAX
      DFB = PLNKUT(HNU / THETA(K), HNUP / THETA(K))
  392 B(K) = DFB * THETA(K)**4
C                                                                              DRAD 363
C                 SET BLACKBODY CONDITIONS
C                                                                              DRAD 365
C     INNER CYLINDRICAL RADIUS NOT ASSUMED ZERO
  480 BBL = 0.
      IF (BCLTAG .LE. 0.0)  GO TO 490
      DFB = PLNKUT(HNU / BCLTAG, HNUP / BCLTAG)
      BBL = BCLTAG**4 * DFB
  490 BBR = 0.
      IF (BCRTAG .LE. 0.0)  GO TO 500
      DFB = PLNKUT(HNU / BCRTAG, HNUP / BCRTAG)
      BBR = BCRTAG**4 * DFB
  500 BBB = 0.0
      IF (BCBTAG .LE. 0.0)  GO TO 510
      DFB = PLNKUT(HNU / BCBTAG, HNUP / BCBTAG)
      BBB = BCBTAG**4 * DFB
  510 BBA = 0.0
      IF (BCATAG .LE. 0.0)  GO TO 520
      DFB = PLNKUT(HNU / BCATAG, HNUP / BCATAG)
      BBA = BCATAG**4 * DFB
  520 CALL DVCHK(KDMY)
      GO TO (522, 521), KDMY
```

```
  522 S1 = 13.0522
      CALL UNCLE
C
C                 FORM ROSSELAND AND PLANCK OPTICAL DEPTHS
C
C     DOUBLE ON STORAGE FOR ABSORPTION COEFFICIENTS, MU, AND LAMBDA
  521 DO  530  I = 1, IMAX
      K = I + 1
      M = K - IMAX
      DO  530  J = 1, JMAX
      FACTOR = 1.
      IF (RPTAG .NE. 0.0)  FACTOR = ROSS(K) / PLANCK(K)
      ROSS(K) = AMAX1(ROSS(K) * RHO(K), 1.E-20)
      PLANCK(K) = AMAX1(PLANCK(K) * RHO(K) * FACTOR, 1.E-20)
C     FORM LAMBDA, MEAN FREE PATH AT CELL EDGES
      IF (I .EQ. 1)  GO TO 525
C     MAY BE ABLE TO SAVE STORAGE BY EQUIVALENCING ALAMH WITH ROSS.
CAVEAT.  LOGIC WOULD BE MORE COMPLEX AND ONE 1-D ARRAY WOULD BE NEEDED.
      DTAUR =    ROSS(K) * DX(I)
      DTAUL =    ROSS(K-1) * DX(I-1)
      IF (ABS(DTAUR - DTAUL) / (DTAUR + DTAUL) .LE. ODDC)  GO TO 523
      ALAMV(K) = AMAX1(1. /   ROSS(K), 1. /   ROSS(K-1))
      GO TO 525
  523 ALAMV(K) = (DX(I) + DX(I-1)) / (DTAUR + DTAUL)
  525 IF (J .EQ. 1)  GO TO 529
      DTAUA =    ROSS(K) * DY(J)
      DTAUB =    ROSS(M) * DY(J-1)
      IF (ABS(DTAUA - DTAUB) / (DTAUA + DTAUB) .LE. ODDC)  GO TO 527
      ALAMH(K) = AMAX1(1. /   ROSS(K), 1. /   ROSS(M))
      GO TO 529
  527 ALAMH(K) = (DY(J) + DY(J-1)) / (DTAUA + DTAUB)
  529 M = M + IMAX
      K = K + IMAX
  530 CONTINUE
C**************************************************************************
C     BEGIN NONEQUILIBRIUM DIFFUSION TREATMENT
C
C     FORM MATRIX ELEMENTS XA, XB, XC, XD, XALP, XGAM
C     THIS SECTION ALSO EXECUTES EQS. 45 AND 46 OF OLIPHANT
C     BOUNDARY CONDITION MODIFIES XB AND XD.
C     THIS CODING ASSUMES DX(I) = X(I+1) - X(I), SAME FOR Y.
      DO  560  I = 1, IMAX
      K = I + 1
      N = K + IMAX
      DO  560  J = 1, JMAX
      XB(K) = 0.
      XD(K) = 0.
      IF (I .EQ. 1)  GO TO 531
      XA(K) = -PUR(I) * RUR(I) * ALAMV(K)
      GO TO 535
  531 XA(K) = 0.0
C     INNER CYLINDRICAL RADIUS ASSUMED ZERO
  535 IF (I .EQ. IMAX)  GO TO 538
  536 XC(K) = -PUR(I) * RUR(I+1) * ALAMV(K+1)
      GO TO 540
  538 XC(K) = 0.0
      IF (BCRTAG .LT. 0.0)  GO TO 540
      BETAR(J) = 1.0 / (2. - EXP(-DX(I) * SQRT(0.75 * ROSS(K)
     2 * PLANCK(K))))
      XB(K) = XB(K) + PUR(I) * 3.E10 * X(I   ) * BETAR(J)
      XD(K) = XD(K) - 4.104E12 * PUR(I) * X(I+1) * BBR
  540 IF (J .EQ. 1)  GO TO 543
      XALP(K) = -PUZ(J) * RUZ(J) * ALAMH(K)
      GO TO 545
  543 XALP(K) = 0.0
```

```
      IF (BCBTAG .LT. 0.0)  GO TO 545
      BETAB(I) = 1.0 / (2. - EXP(-DY(1) * SQRT(0.75   ROSS(K)
     2 * PLANCK(K))))
      XB(K) = XB(K) + PUZ(1) * 1.5E10 * BETAB(I)
      XD(K) = XD(K) - PUZ(1) * 2.052E12 * BBB
  545 IF (J .EQ. JMAX)  GO TO 548
  546 XGAM(K) = -PUZ(J) * RUZ(J+1) * ALAMH(N)
      GO TO 549
  548 XGAM(K) = 0.0
      IF (BCATAG .LT. 0.0)  GO TO 549
      BETAA(I) = 1.0 / (2. - EXP(-DY(J) * SQRT(0.75 * ROSS(K)
     2 * PLANCK(K))))
      XB(K) = XB(K) + PUZ(J) * 1.5E10 * BETAA(I)
      XD(K) = XD(K) - PUZ(J) * 2.052E12 * BBA
  549 XB(K) = XB(K) + 3.E10*PLANCK(K) - XA(K) - XC(K) - XALP(K) -XGAM(K)
      XD(K) = XD(K) - 4.104E12 * PLANCK(K) * B(K)
C  * * * * * * * * * * * * * * * * * * * * * * * *
C     INITIAL ERAD(K)=0. FOR LOW FLUX AND B(K)*137. FOR HIGH FLUX
      ERAD(K) = B(K) * 137.
C  * * * * * * * * * * * * * * * * * * * * * * * *
      IF (IMPTAG .EQ. 0 .OR. MFTAG .NE. 0)  GO TO 559
C     FULLY IMPLICIT ADJUSTMENT OF XB AND XD
C     VDOT, DE(M)/DT, Q, PHIN, AND SO FORTH NOT YET AVAILABLE.
      S1 = 13.0559
      CALL UNCLE
      XB(K) = XB(K)
      XD(K) = XD(K)
  559 K = K + IMAX
      N = N + IMAX
  560 CONTINUE
C     FIRST PASS -- P. 16, EQS. 47-49 OF OLIPHANT
      DO  570  K = 2, KMAX
      M = K - IMAX
      XB(K) = XB(K) - XALP(K) * XGAM(M) - XA(K) * XC(K-1)
      XGAM(K) = XGAM(K) * CMXK / XB(K)
      XC(K) = XC(K) * CMXK / XB(K)
  570 CONTINUE
      CALL DVCHK(KDMY)
      GO TO (572, 573), KDMY
  572 S1 = 13.0572
      CALL UNCLE
  573 IF(AMOD(CYCLE,PRINTL). NE. 0.) GO TO 580
      WRITE(6,4) CYCLE , T , DT
      WRITE (6,5)
      DO  575  K = 2, KMAX
  575 WRITE (6,6) K, XA(K), XB(K), XC(K), XD(K), XALP(K), XGAM(K), B(K),
     2 ROSS(K), PLANCK(K)
  580 ITER = 1
C     SECOND PASS -- EQS. 50, 51 OF OLIPHANT
  590 DO  600  K = 2, KMAX
      M = K - IMAX
      N = K + IMAX
      XH = -XD(K) + XALP(K) * XC(M) * ERAD(M+1) + XA(K) * XGAM(K-1) *
     2 ERAD(N-1) + (CMXK - 1.) * XB(K) / CMXK * (XGAM(K) * ERAD(N) +
     3 XC(K) * ERAD(K+1))
      XG(K) = (XH - XALP(K) * XG(M) - XA(K) * XG(K-1)) / XB(K)
  600 CONTINUE
C     BACKWARD PASS -- EQ. 52 OF OLIPHANT
      ERROR = 0.
      EMIN = 1.E20
      DO  620  L = 2, KMAX
      K = KMAXA + 1 - L
      N = K + IMAX
      ENEW = CMXOM * (XG(K) - XGAM(K) * ERAD(N) - XC(K) * ERAD(K+1)) +
     2 (1. - CMXOM) * ERAD(K)
```

```
C     MAY BE TOO SEVERE FOR CELLS WITH VERY LITTLE OF THE TOTAL ENERGY
      EMIN = AMIN1(EMIN, ENEW)
      ERRT = ABS((ENEW - ERAD(K)) / ENEW)
      IF (ERRT .LE. ERROR)  GO TO 619
      ERROR = ERRT
      KME = K
      EME = ENEW
  619 ERAD(K) = ENEW
  620 CONTINUE
      IF(AMOD(CYCLE,PRINTS).EQ.0.)
     1WRITE (6,8)  ITER, ERROR, KME, EME
      IF(AMOD(CYCLE,PRINTL).NE.0.) GO TO  635
      IF (DBGPRT .EQ. 0.0)  GO TO 635
      WRITE (6,9)
      WRITE (6,11)  (XG(K), K=2,KMAX)
      WRITE (6,10)
      WRITE (6,11)  (ERAD(K), K=2,KMAX)
  635 GO TO 640
      S1 = 13.0635
      CALL UNCLE
  640 CALL DVCHK(KDMY)
      GO TO (641, 645), KDMY
  641 S1 = 13.0641
      CALL UNCLE
  645 ITER = ITER + 1
      IF (ITER .LE. ITRMAX)  GO TO 648
      S1 = 13.0648
      CALL UNCLE
  648 IF (ERROR .GT. ERRCRT)  GO TO 590
C     CALCULATE FLUXES, USING XA AND XB FOR STORAGE
      DO  680  I = 1, IMAX
      K = I + 1
      M = K - IMAX
      DO  680  J = 1, JMAX
      IF (J .EQ. 1)  GO TO 650
      XA(K) = RUZ(J) * ALAMH(K) * (ERAD(M) - ERAD(K))
      GO TO 655
  650 IF (BCBTAG)  651, 652, 652
  651 XA(K) = 0.0
      GO TO 655
  652 XA(K) = 2.052E12 * BBB - 1.5E10 * ERAD(K) * BETAB(I)
  655 IF (I .EQ. 1)  GO TO 660
      XB(K) = RUR(I) * ALAMV(K) * (ERAD(K-1) - ERAD(K))
      GO TO 665
  660 XB(K) = 0.0
  665 K = K + IMAX
      M = M + IMAX
  680 CONTINUE
      DO  690  I = 1, IMAX
      K = I + 1
      N = K + IMAX
      DO  690  J = 1, JMAX
      FABV = XA(N)
      IF (J .NE. JMAX)  GO TO 683
      IF (BCATAG)  681, 682, 682
  681 FABV = 0.0
      GO TO 683
  682 FABV = -2.052E12 * BBA + 1.5E10 * ERAD(K) * BETAA(I)
  683 FRT = XB(K+1)
      IF (I .NE. IMAX)  GO TO 686
      IF (BCRTAG)  684, 685, 685
  684 FRT = 0.0
      GO TO 686
  685 FRT = -2.052E12 * BBL + 3.0E10 * ERAD(K) * X(IMAX ) * BETAR(J)
  686 ER(K) = ER(K) + (XA(K)-FABV) * TAU(I) + (XB(K)-FRT) * PIDY * DY(J)
```

```
      K = K + IMAX
      N = N + IMAX
  690 CONTINUE
C
C                   OPTIONAL EDIT OF FLUX AND ENERGY CHANGE            DRAD 555
C
      IF(AMOD(CYCLE,PRINTL).NE.0.) GO TO 1020                          DRAD 557
      IF (DBGPRT .EQ. 0.0)  GO TO 1020
      WRITE (6,7)
      DO  1010  K = 2, KMAX
 1010 WRITE (6,6)  K, XA(K), XB(K), ER(K)
C
C     ADVANCE FREQ, STORE EMERGENT FLUX, TEST FOR COMPLETION OF GROUPS DRAD 576
C                                                                      DRAD 577
 1020 CALL DVCHK (KDMY)                                                DRAD 578
      GO TO (1050,1040), KDMY
 1040 HNUP=HNU
      HNUP4=HNU4
      IF(IHNU-NHNU)360,1060,1050                                       DRAD 583
C***********************************************************************DRAD 586
C                                                                     *DRAD 587
C                  E N D   F R E Q U E N C Y   L O O P                *DRAD 588
C                                                                     *DRAD 589
C***********************************************************************DRAD 590
 1050 S1 = 13.1050                                                     DRAD 591
      CALL UNCLE                                                       DRAD 592
C     ITERATE ON TEMPERATURE                                           DRAD 593
 1060 GO TO (1061, 1065), NVEZ                                         DRAD 594
 1061 NVEZ = 2                                                         DRAD 595
      VEZ = NVEZ                                                       DRAD 596
      NY = NVEZ                                                        DRAD 597
      IHNU = 0
      DO  1062  K = 2, KMAX
C     WORK, SOURCE TERMS OMITTED
      BNTH = THETA(K) + ER(K) * TRAD / (AMX(K) * XCV(K))
      OLDTH(K) = THETA(K)
      THETA(K) = 0.5 * (OLDTH(K) + BNTH)
 1062 CONTINUE
      IF (MFTAG .EQ. 0)  CALL KAPPA
      GO TO 200                                                        DRAD 605
 1065 IF (ITAG .EQ. 0)  GO TO 1067
      DO  1066 K = 2, KMAX
 1066 THETA(K) = OLDTH(K)
 1067 RETURN
      END
```

SECTION V

THE METHOD OF CHARACTERISTICS IN CYLINDRICAL GEOMETRY

5.1. INTRODUCTION

As a first step in the development of a true two-dimensional transport code, a subprogram called TRAN2 has been written to treat the case in which retardation and scattering can be ignored. TRAN2 is designed to operate in HECTIC, which is a code that calculates hydrodynamical problems having axial symmetry, and which normally uses the diffusion approximation for computing the rate of flow of radiation.

Consider a cylindrical region of outer radius R and altitude Z. Assume that the axis of the cylinder is an axis of symmetry for all the properties of the material contained in the cylinder so that all quantities of interest can be expressed as functions of two cylindrical coordinates, the distance r from the axis and the altitude z above the bottom.

In TRAN2, the transport equation is integrated along a system of characteristic lines, called rays, which are distributed throughout the system in a more or less uniform manner.

5.2. THE LOCAL COORDINATE SYSTEM

Given any point P in the system, let there be three associated unit vectors: $\vec{k}$, a vector which is parallel to the axis of the system and which points in the same direction, called "upward," for all points P; $\vec{j}$, a unit vector parallel to the radial direction at P; and $\vec{i} = \vec{j} \times \vec{k}$.

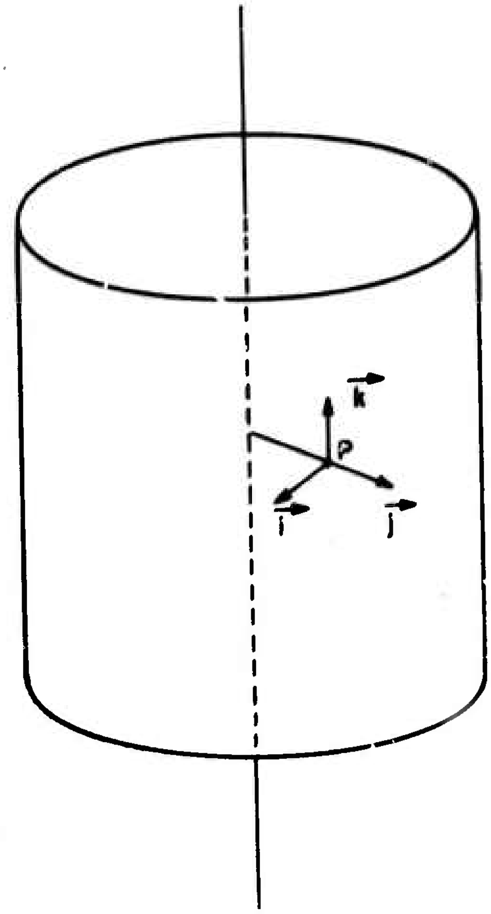

Figure 12. Coordinate Vectors

5.3. DISTRIBUTION OF RAYS

A ray is a directed line segment

$$L: \vec{r}(s) = s\vec{\Omega} + \vec{p} \quad \text{for} \quad -S \le s \le S$$

where $\vec{\Omega}$ is a unit vector called the direction of L and $\vec{p}$ is the midpoint of L. There are groups, called combs, of rays lying in the same vertical plane and having the same length 2S and direction $\vec{\Omega}$. The midpoints of the rays of a comb lie in a vertical line at altitudes $z = 0, \Delta z, 2\Delta z, \ldots,$ where $\Delta z = Z/m$, m being an integer, is the same for all combs. If a comb is thought of as going to infinity in both directions, then the reflection of a comb is the same in both ends of the system and is another comb

with the same midpoints and the same $\vec{\Omega} \times \vec{k}$. Thus, if a ray strikes the end of the system, its reflection is a ray in the reflected comb.

It will be convenient to consider groups of rays of another type, called grids (see Section 3.3). A different definition is given there but they turn out to be equivalent. A grid consists of all rays for which $\Omega \cdot k$ has a given value μ. In view of the symmetry of the system, it can be assumed that the midpoints of all rays of a grid lie in the same vertical half-plane and that their directions all have positive projections on the same normal of the half-plane, in which case they will be parallel to each other. The rays of a comb, being parallel, all lie in the same grid and are separated by a distance of $\Delta z(1 - \mu^2)^{1/2}$, where $\mu = \vec{\Omega} \cdot \vec{k}$. The combs that make up the grid are to have a constant separation $d(\Omega)$ which will generally differ from $\Delta z(1 - \mu^2)^{1/2}$, so that the lattice of points in which the rays of a grid intersect a mutually perpendicular plane will be rectangular.

By considering all rays together, it ought to be possible to infer the essential features of the distribution of the directions they assume at some particular radial distance r from the axis of the system, when the angles at which rays penetrate a cylindrical strip of radius r and altitude $\Delta z = Z/m$ are given. The reasons are clear. First, this set of angles is the same for all such strips because the distribution of rays is periodic with period $\Delta z \vec{k}$. Consequently, it suffices to specify them for one arbitrarily chosen strip. Second, because of the axial symmetry of the system, rotation of the ray about the axis leaves the ray in essentially the same position. Third, it is assumed that Δz is so small that moving a ray up or down through such a distance will not have a significant effect on the accuracy of the results.

In terms of the local coordinate vectors $\vec{i}$, $\vec{j}$, $\vec{k}$ associated with some particular point on a ray, the direction $\vec{\Omega}$ of the ray can be expressed as $\vec{\Omega} = \mu\vec{k} + (1 - \mu^2)^{1/2}(\vec{i}\sin\phi + \vec{j}\cos\phi) = \mu\vec{k} + \lambda\vec{i} + \eta\vec{j}$, where $\mu^2 + \lambda^2 + \eta^2 = 1$, and, because of symmetry, $0 \le \phi \le \pi$ and $0 \le \lambda \le 1$.

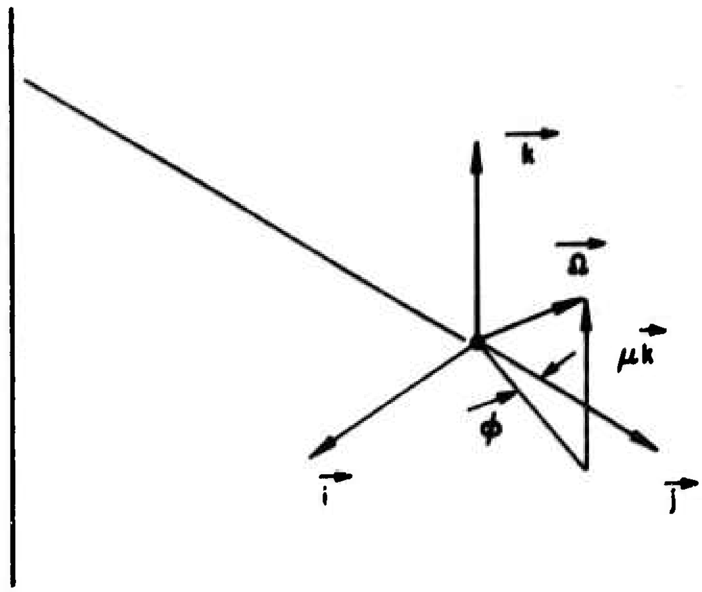

Figure 13. Components of Ω

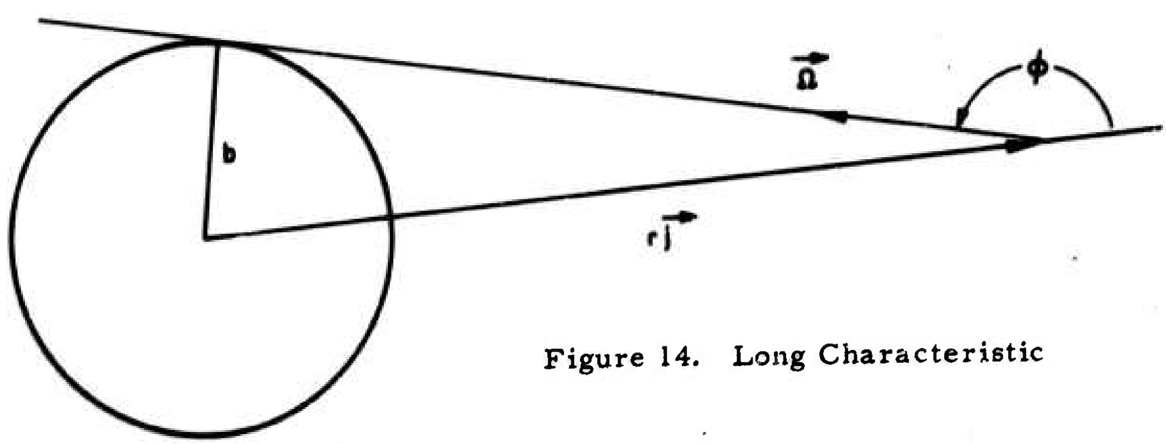

Figure 14. Long Characteristic

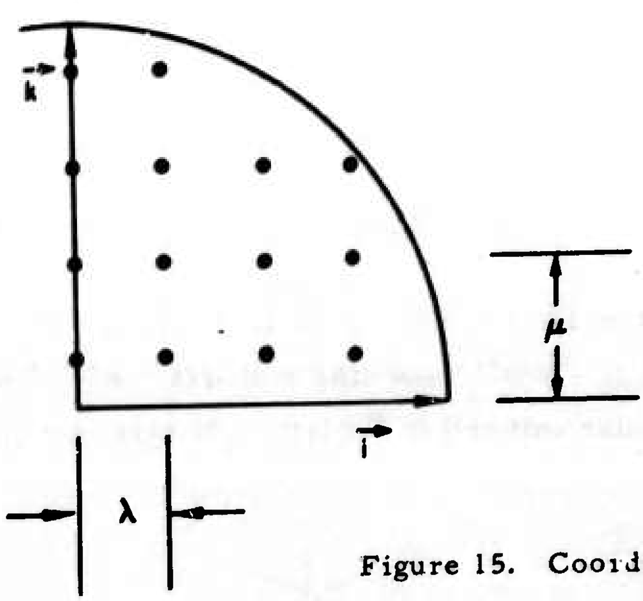

Figure 15. Coordinates μ and λ

As the point moves along the ray in the direction $\vec{\Omega}$, μ is fixed, but unless $\mu^2 = 1$, ϕ decreases. It can be seen that $\sin\phi = b/r$, where b is the distance between the ray and the axis. (See Figs. 13 and 14.)

The projection of the direction $\vec{\Omega}$ of a ray in the i-k plane is $\vec{\Omega} - \vec{\Omega} \cdot \vec{j}\vec{j} = \mu\vec{k} + \lambda\vec{i} = \mu\vec{k} + (1 - \mu^2)^{1/2} \sin\phi\vec{i}$. The distribution of directions of rays that intersect a given strip of radius r and altitude z will be isotropic if the distribution of their projections is uniform over the unit disk in the i-k plane. (See Fig. 15.) In such a λ, μ plot, the rays of one grid will lie in a horizontal line $\mu = \vec{\Omega} \cdot \vec{k}$ = const. As r changes, μ remains fixed, and since $\lambda = (1 - \mu^2)^{1/2}$ (b/r), λr remains fixed also. Given two radii, r_1 and r_2 with $r_1 < r_2$, a ray with $\lambda = \lambda_2$ at $r = r_2$ will have $\lambda = \lambda_2 r_2/r_1$ at $r = r_1$ (assuming that the distance b from the ray to the axis of the system is no greater than r_1), so that on a plot of projections like Fig. 15, moving from r_2 to r_1 will cause a dilation of the pattern of projections by a factor of r_2/r_1. Those projections for which $\lambda_2^2 > 1 - \mu^2$ correspond to points that fall outside the unit circle, but they are associated with the rays for which $r_1 < b \leq r_2$. At any rate, the dilation is constant for all directions, so a distribution that is uniform at r_2 will, of course, remain uniform at r_1. Unfortunately, the density of directions is much reduced at smaller radii, which is a basic difficulty with the method.

The method that is used in TRAN2 to obtain a uniform distribution of projections on the unit disk is to choose N equally spaced values of μ,

$$\mu = \frac{2n - 1}{2N}, \qquad = 1, 2, \ldots, N$$

and for each μ to let $\lambda = Cj$, $j = 0, 1, 2, \ldots, j < (1 - \mu^2)^{1/2}/C$, at $r = R$. Then $b = RCj/(1 - \mu^2)^{1/2}$ and $d(\mu) = RC/(1 - \mu^2)^{1/2}$ are the dimensions of the rectangular unit cell in the lattice of rays in a grid.

5.4. CALCULATION OF INTENSITIES

Let V_i denote the volume of zone i of the mesh imposed on the hydrodynamical calculation by HECTIC; let L_i denote the sum of the lengths of segments of rays intersected by zone i; and set $A_i = 4\pi V_i / L_i$. Then A_i should not vary much from zone to zone. Radical variations in A_i indicate that the density of rays in the grid is too low.

The quantity A_i has the dimensions of area and is, in a way, taken to be a measure of the cross section of a beam associated with the ray. The quantity that is calculated at each point along a ray is the rate of flow of energy through the beam that the ray represents. In zone i this is

$$J(s) = J(o)\, e^{-\sigma_i s} + A_i S_i\, s\, \frac{1 - e^{-\sigma_i s}}{\sigma_i s}$$

assuming that the source S_i and volume coefficient of absorption σ_i are constants. The rate of energy deposition in zone i is then

$$\frac{dE_i}{dt} = \sigma_i \sum \int_o^{\ell} J(s)ds = J_{io} \sum (1 - e^{-\sigma_i \ell}) + A_i S_i \sum \ell \left(1 - \frac{1 - e^{-\sigma_i \ell}}{\sigma_i \ell}\right)$$

where the summations range over rays that intersect zone i. The rate of emission is, of course, $A_i S_i L_i = 4\pi S_i V_i$.

The rate at which radiation passes through a surface is just the sum of the J's over all points at which rays intersect the surface.

It remains to discuss the calculation of J at the point at which a ray enters the system. At the curved outer surface, it is easy to see what to do. The boundary condition must specify for each strip of altitude ΔZ on the outer surface what the incident radiant intensity is as a function of direction. By using μ and λ as coordinates, the direction of each incoming ray may be projected as a point on the unit disk, as was done in Fig. 15. The area of the disk is then subdivided so that in each subdivision

there is one point more or less in the center. The initial energy J carried by a given ray is then

$$J = 2\pi R \, \Delta z \, I^*$$

where I^* is the integral of the intensity over the solid angle of directions that are projected on the subdivision of the unit disk associated with the given ray.

In TRAN2, only isotropic boundary radiation is presently handled, so $J = (4\pi^2 R \, \Delta z \, I)/N_o$, where I is the mean intensity on the strip through which the ray enters and N_o is the number of grids, or, in other words, the number of rays entering through a strip of altitude Δz.

The situation at the ends of the cylindrical system could be quite difficult to treat by a method analogous to the one just described for the curved surface. TRAN2 treats two cases: (1) no incident radiation, and (2) perfect reflection. But the way to treat a boundary condition like that corresponding to an incident laser beam is to introduce an entirely new set of rays which have no role in the calculation of radiative transfer of energy within the system but simply provide channels for the deposition of external radiation.

5.5. THICK ZONES

Experience (with SPUTTER* for example) has shown that the method of characteristics must be applied with care when the distance between zone boundaries becomes more than a few times the length of a mean free path. In some cases, it might be impossible to determine the distribution of radiation within a thick zone because of loss of information due to mixing, and a reduction of the mesh spacing would be necessary. Frequently, the diffusion approximation will give satisfactory results without

*Freeman, B.E., and C.G. Davis, "Fireball Phenomenology and Code Development. Vol. III, "SPUTTER Subroutines for Radiation Transport in Spheres," Air Force Weapons Laboratory Report AFWL-TR-65-143, General Atomic Division, General Dynamics Corporation, August, 1965.

refinement of the spatial mesh when the transport approximation used in TRAN2, which assumes constant source strengths throughout individual zones, does not. For this reason, it will be necessary to treat thick zones by a special method. An application of the diffusion approximation to thick zones is being developed as follows. When the number of mean free paths between the boundaries of a zone is above a critical value specified by input, that zone is classified as thick. When two thick zones have a common boundary surface, the rays intersecting that surface are ignored and the diffusion approximation is applied to calculate the rate of transfer of radiant energy between them. When a thick zone has a boundary in common with an ordinary one, the energy that it radiates through that surface is calculated and divided uniformly among the rays that pass through it. Similarly, the energy coming in along these rays from the ordinary zone is all dumped into the thick zone, all transmission factors being neglected.

SECTION VI

FREQUENCY-AVERAGED TRANSMISSION FUNCTIONS

6.1 INTRODUCTION

In this section a technique is proposed for the implementation of the treatment of the characteristic equation of radiative transport theory suggested by B. E. Freeman (Ref. 1). A review of the formulation is presented first, both to establish notation and to describe certain modifications made in the originally proposed formulation.

The characteristic equation for the intensity $I(\underline{\Omega}, \tau, \nu)$ of radiation of frequency ν in a direction $\underline{\Omega}$ at optical depth τ is

$$\frac{d}{d\tau} I(\underline{\Omega}, \tau, \nu) + I(\underline{\Omega}, \tau, \nu) = B(\underline{\Omega}, \theta, \nu) \tag{69}$$

where $B(\underline{\Omega}, \theta, \nu)$ is the blackbody source intensity for temperature θ:

$$B(\underline{\Omega}, \theta, \nu)d\nu = \frac{2h\nu^3}{c^2} \left(e^{h\nu/\theta} - 1\right)^{-1} d\nu \tag{70}$$

It is necessary to evaluate the integral of $I(\underline{\Omega}, \tau, \nu)$ over prescribed intervals of $\underline{\Omega}$, r, and ν. In systems with plane or spherical symmetry, the intensity as well as the source is independent of azimuth, so that the integration over this part of $\underline{\Omega}$ may be performed at once. Integration over μ, the cosine of the angle between the ray and the normal direction $\underline{r}$, is carried out after integration along the ray, and is not discussed in this report. For the sake of brevity, the argument μ for the intensity and source functions will be suppressed. The element of optical depth is defined by

$$d\tau = \sigma(\theta, \rho, \nu)ds \tag{71}$$

where the cross section

$$\sigma(\theta,\rho,\nu) = \rho\kappa'(\theta,\rho,\nu) = \rho\kappa(\theta,\rho,\nu)(1 - e^{-h\nu/\theta}) \tag{72}$$

includes the usual correction for induced emission, and the element of length along the ray is defined by

$$ds = \frac{dr}{\mu} \tag{73}$$

in plane geometry, while in spherical geometry with

$$x = r\mu, \quad y = r\sqrt{1 - \mu^2} \tag{74}$$

$$ds = dx \tag{75}$$

Equation (69) therefore becomes

$$\frac{d}{d\tau} I(\tau, \nu) + I(\tau, \nu) = B(\theta, \nu) \tag{76}$$

with

$$B(\theta, \nu)d\nu = \frac{4\pi h\nu^3}{c^2} (e^{h\nu/\theta} - 1)^{-1} d\nu \tag{77}$$

If the variable $u = h\nu/\theta$ is introduced, then Eq. (77) is equivalent to

$$B(\theta, u)du = \frac{4\pi\theta^4}{h^3 c^2} \frac{u^3}{e^u - 1} du \tag{78}$$

In terms of the normalized Planck function,

$$W_1(u) = \frac{15}{\pi^4} \frac{u^3}{e^u - 1} \tag{79}$$

$$B(\theta, u)du = \frac{ac}{2} \theta^4 W_1(u)du \tag{80}$$

where

$$\frac{ac}{2} = 2\sigma = \frac{4\pi^5}{15h^3 c^2} \tag{81}$$

is twice the Stefan-Boltzmann constant; if θ is in ev units, a = 137.20.

For later reference, the functions

$$f(u) = \int_u^\infty W_1(u')du' \tag{82}$$

$$g(u) = \frac{u}{4} W_1(u) \tag{83}$$

and

$$W_2(u) = \left(\frac{df}{du} + \frac{dg}{du}\right) = \frac{15}{4\pi^4} \frac{u^4 e^u}{(e^u - 1)^2} \tag{83a}$$

are needed. For example,

$$\int_{u_1}^{u_2} B(\theta, u)du = \frac{ac}{2} \theta^4 \left[f(u_1) - f(u_2)\right] \tag{84}$$

$$\int_{u_1}^{u_2} \frac{dB}{d\theta} du = 2\,ac\,\theta^3 \int_{u_1}^{u_2} W_2(u)du = 2\,ac\,\theta^3 \left[f(u_1) - f(u_2) + g(u_1) - g(u_2)\right] \tag{85}$$

It is customary to absorb a factor 1/c in the definitions of B and I, in which case the factor c does not appear in Eqs. (80), (84), and (85).

Since the temperature varies with position, and therefore with optical depth, the notation $B(\tau, \nu)$ may be introduced in place of $B(\theta(\tau), \nu)$. The integral with respect to τ of Eq. (76) over an interval $\tau_o < \tau < \tau_1$ is then

$$I(\tau_1, \nu) = I(\tau_o, \nu)\, e^{-(\tau_1 - \tau_o)} + \int_{\tau_o}^{\tau_1} B(\tau, \nu)\, e^{-(\tau_1 - \tau)}\, d\tau \tag{86}$$

Assume that $B(\tau, \nu)$ is linear in τ over this interval with slope $\partial B/\partial\tau$; then

$$I(\tau_1, \nu) = B(\tau_1, \nu) - \frac{\partial B}{\partial \tau} + \left[I(\tau_o, \nu) - B(\tau_o, \nu) + \frac{\partial B}{\partial \tau}\right] e^{-(\tau_1 - \tau_o)} \tag{87}$$

The first two terms on the right side of Eq. (87) represent the diffusive intensity. The quantity in brackets represents the streaming (nondiffusive) part of the intensity at τ_o, which is attenuated by an exponential "transmission function" on the way to τ_1.

6.2 FREQUENCY AVERAGING FOR THE TRANSPORT EQUATION

The problem to be discussed is the way in which the integration of Eq. (87) over the frequency ν should be carried out. The simplest approach is just to substitute frequency-averaged optical depths for the variable τ in Eq. (87) The appropriate average for $\partial B/\partial\tau$ is $\partial B/\partial\tau^R$, where τ^R is the Rosseland mean optical depth (see Eq. (93) below). However, the Rosseland mean is frequently inappropriate for use in the exponential transmission function. The Planck mean defined by Eq. (94) below is valid in the limit of an extremely thin region ($\tau^P << 1$), while the Rosseland mean is preferable in the thick limit, where the transmission function is relatively small anyway. Other means can be constructed from the Planck and Rosseland means, such as the geometric mean $\sqrt{\tau^P\tau^R}$ or the mean proposed by Sampson (Ref. 2):

$$\bar{\tau} = \left(\frac{b + \tau^R}{b + \tau^P}\right)\tau^P$$

where b is an adjustable parameter of order unity. Without doubt, such means, particularly the last-mentioned, are useful expedients in many cases, but experience has shown that they must be used with some caution. In this report, Eq. (87) is treated in a more systematic manner, as in Ref. 1.

The medium is divided for computational purposes into zones by interfaces whose coordinates are denoted by r_i. A subscript i-1, i, i+1, etc., on a quantity implies that the quantity is to be evaluated on an interface, while a subscript such as i-1/2 or i+1/2 implies evaluation either for the zone as a whole or for an interior point in the zone. This point will be assumed to be the midpoint of the ray, so that

$$s_i - s_{i-1/2} = s_{i-1/2} - s_{i-1} = \delta_{i-1/2} \tag{88}$$

is the half-width of zone i-1/2, measured along the ray. In particular, the density $\rho_{i-1/2}$ and temperature $\theta_{i-1/2}$ are given quantities associated with each zone or zone midpoint, and it is desired to calculate intensities $(I_i(\nu)$ at the interfaces. It is therefore natural to carry out the integration of Eq. (86) in half-zone steps, within each of which $B(\tau, \nu)$ can be assumed linear in τ. Thus,

$$I(\tau_i, \nu) = B(\tau_i, \nu) - \left(\frac{\partial B}{\partial \tau}\right)_i + \left[I(\tau_{i-1/2}, \nu) - B(\tau_{i-1/2}, \nu) + \left(\frac{\partial B}{\partial \tau}\right)_i \right] e^{-(\tau_i - \tau_{i-1/2})} \tag{89}$$

$$I(\tau_{i-1/2}, \nu) = B(\tau_{i-1/2}, \nu) - \left(\frac{\partial B}{\partial \tau}\right)_{i-1} + \left[I(\tau_{i-1}, \nu) - B(\tau_{i-1}, \nu) + \left(\frac{\partial B}{\partial \tau}\right)_{i-1} \right] e^{-(\tau_{i-1/2} - \tau_{i-1})} \tag{90}$$

In order to carry out the integration of Eqs. (89) and (90) over frequency, three further assumptions are required. First, it will be assumed that cross sections have a piecewise-constant dependence upon position. This is done for simplicity, since it provides for a piecewise-linear relationship between position and optical depth which is more convenient than a quadratic or other type relationship and is no less consistent with the available information. Second, the cross sections will be evaluated at, or at least associated with, zone boundaries rather than zone midpoints (using, for example, an interpolated density and temperature at each boundary). This choice is made primarily for experimental reasons, but is guided also by the physical consideration that the opacity is ultimately needed for the calculation of radiative flux across zone boundaries, and is in this sense most naturally defined as a boundary-centered, rather than a zonal, quantity. There is probably no single best method for evaluating opacity at

zone interfaces; in some cases it might suffice to use the lesser of the adjacent zone opacities. If interpolation is to be done, however, it is simpler and probably less dangerous to interpolate temperatures and densities than to interpolate zonal opacities directly. The formulation adopted is in any case quite general. The most economical method would prescribe the cross section as constant from one midpoint to the next, but allowance can also be made for possible interface discontinuity.

The third assumption is made purely for convenience. It will be assumed that $I(\tau, \nu)$ has a frequency dependence within each group proportional to that of $B(\tau, \nu)$. The validity of this assumption depends on the variation of opacity within the group, and cannot be taken for granted in a few-group calculation.

The following definitions are needed:

$$B_{ij} = \int_{\nu_j}^{\nu_{j+1}} B(\theta_i, \nu) d\nu, \text{ the group source} \tag{91}$$

$$I_{ij} = \int_{\nu_j}^{\nu_{j+1}} I(\tau_i, \nu) d\nu, \text{ the group intensity} \tag{92}$$

$$\sigma_{ij}^{R} = \frac{dB_{ij}/d\theta}{\displaystyle\int_{\nu_j}^{\nu_{j+1}} \frac{1}{\sigma(\theta_i, \rho_i, \nu)} \left(\frac{dB}{d\theta}\right)_{\theta_i} d\nu}, \text{ the group Rosseland mean cross section} \tag{93}$$

$$\sigma_{ij}^{P} = \int_{\nu_j}^{\nu_{j+1}} B(\theta_i, \nu)\, \sigma(\theta_i, \rho_i, \nu) d\nu / B_{ij}, \text{ the group Planck mean} \tag{94}$$

$$S_{ij}(\delta) = \int_{\nu_j}^{\nu_{j+1}} B(\theta_i, \nu) e^{-\sigma(\theta_i, \rho_i, \nu)\delta} d\nu / B_{ij}, \text{ the Planck transmission function} \tag{95}$$

and

$$T_{ij}(\delta) = \int_{\nu_j}^{\nu_{j+1}} \frac{1}{\sigma(\theta_i, \rho_i, \nu)} \left(\frac{dB}{d\theta}\right)_{\theta_i} e^{-\sigma(\theta_i, \rho_i, \nu)\delta} \, d\nu \Big/ \left(\frac{1}{\sigma^R_{ij}} \frac{dB_{ij}}{d\theta}\right) \tag{96}$$

the Rosseland transmission function.

Equations (89) and (90) then may be integrated over the j^{th} frequency group; notation is further specified as follows:

$$I_{ij} = \overline{B}_{ij} - \left(\frac{dB}{d\tau^R}\right)_{ij} + (I_{i-1/2,j} - \overline{B}_{i-1/2,j})\, S^-_{ij}(\delta_{i-1/2}) + \left(\frac{dB}{d\tau^R}\right)_{ij} T^-_{ij}(\delta_{i-1/2}) \tag{97}$$

$$I_{i-1/2,j} = \overline{B}_{i-1/2,j} - \left(\frac{dB}{d\tau^R}\right)_{i-1,j} + (I_{i-1,j} - \overline{B}_{i-1,j}) S^+_{i-1,j}(\delta_{i-1/2}) + \left(\frac{dB}{d\tau^R}\right)_{i-1,j} T^+_{i-1,j}(\delta_{i-1/2}) \tag{98}$$

Since I is needed only on interfaces, $I_{i-1/2,j}$ may be eliminated from Eqs. (97) and (98):

$$I_{ij} = \overline{B}_{ij} + \left\{(I_{i-1,j} - \overline{B}_{i-1,j})\, S^+_{i-1,j}(\delta_{i-1/2}) - \left(\frac{dB}{d\tau^R}\right)_{i-1,j} \left[1 - T^+_{i-1,j}(\delta_{i-1/2})\right]\right\} S^-_{ij}(\delta_{i-1/2}) - \left(\frac{dB}{d\tau^R}\right)_{ij} \left[1 - T^-_{ij}(\delta_{i-1/2})\right] \tag{99}$$

It remains to discuss the definitions of the quantities θ_i, ρ_i, $\overline{B}_{ij}$, and $(dB/d\tau^R)_{ij}$. The interface temperature may be defined by some mean value such as

$$\theta_i = \left(\frac{\theta^4_{i-1/2} + \theta^4_{i+1/2}}{2}\right)^{1/4} \tag{100}$$

$$T_{ij}(\delta) = \int_{\nu_j}^{\nu_{j+1}} \frac{1}{\sigma(\theta_i, \rho_i, \nu)} \left(\frac{dB}{d\theta}\right)_{\theta_i} e^{-\sigma(\theta_i, \rho_i, \nu)\delta} \, d\nu \Big/ \left(\frac{1}{\sigma^R_{ij}} \frac{dB_{ij}}{d\theta}\right) \tag{96}$$

the Rosseland transmission function.

Equations (89) and (90) then may be integrated over the j^{th} frequency group; notation is further specified as follows:

$$I_{ij} = \overline{B}_{ij} - \left(\frac{dB}{d\tau^R}\right)_{ij} + (I_{i-1/2,j} - \overline{B}_{i-1/2,j}) S^-_{ij}(\delta_{i-1/2})$$
$$+ \left(\frac{dB}{d\tau^R}\right)_{ij} T^-_{ij}(\delta_{i-1/2}) \tag{97}$$

$$I_{i-1/2,j} = \overline{B}_{i-1/2,j} - \left(\frac{dB}{d\tau^R}\right)_{i-1,j} + (I_{i-1,j} - \overline{B}_{i-1,j}) S^+_{i-1,j}(\delta_{i-1/2})$$
$$+ \left(\frac{dB}{d\tau^R}\right)_{i-1,j} T^+_{i-1,j}(\delta_{i-1/2}) \tag{98}$$

Since I is needed only on interfaces, $I_{i-1/2,j}$ may be eliminated from Eqs. (97) and (98):

$$I_{ij} = \overline{B}_{ij} + \Big| (I_{i-1,j} - \overline{B}_{i-1,j}) S^+_{i-1,j}(\delta_{i-1/2})$$
$$- \left(\frac{dB}{d\tau^R}\right)_{i-1,j} \left[1 - T^+_{i-1,j}(\delta_{i-1/2})\right] \Big| S^-_{ij}(\delta_{i-1/2})$$
$$- \left(\frac{dB}{d\tau^R}\right)_{ij} \left[1 - T^-_{ij}(\delta_{i-1/2})\right] \tag{99}$$

It remains to discuss the definitions of the quantities θ_i, ρ_i, $\overline{B}_{ij}$, and $(dB/d\tau^R)_{ij}$. The interface temperature may be defined by some mean value such as

$$\theta_i = \left(\frac{\theta^4_{i-1/2} + \theta^4_{i+1/2}}{2}\right)^{1/4} \tag{100}$$

which is used in MOTET. Again, no single prescription can be expected to represent all cases equally well. Provision should be made for alternative methods in special cases; one such method would be use of the zone temperatures on each side of the interface. The + and - superscripts on σ^R, S, and T indicate possible use of such a discontinuous interface treatment (for temperature, density, or both).

The interface density may be evaluated either by position interpolation or by use of a mean value such as the ratio of the combined masses of the two zones to their combined volume. Again, provision for a discontinuity at the interface is desirable.

Simple and consistent definitions of $\overline{B}_{ij}$ and $(dB/d\tau^R)_{ij}$ are obtained by use of source functions evaluated at zone temperatures with Rosseland optical depth interpolation:

$$\left(\frac{dB}{d\tau^R}\right)_{ij} = \frac{B_{i+1/2,j} - B_{i-1/2,j}}{\sigma_{ij}^{R+}\,\delta_{i+1/2} + \sigma_{ij}^{R-}\,\delta_{i-1/2}} \tag{101}$$

$$\overline{B}_{ij} = B_{i-1/2,j} + \left(\frac{dB}{d\tau^R}\right)_{ij} \sigma_{ij}^{R-}\,\delta_{i-1/2} = B_{i+1/2,j} - \left(\frac{dB}{d\tau^R}\right)_{ij} \sigma_{ij}^{R+}\,\delta_{i+1/2} \tag{102}$$

It should be noted that both $\overline{B}_{ij}$ and $(dB/d\tau^R)_{ij}$ are single-valued, regardless of whether or not σ_{ij}^R is, and further that $\overline{B}_{ij}$ must be evaluated by means of Eq. (102), and not evaluated at the interface temperature θ_i. The latter procedure would yield B_{ij} as defined in Eq. (91), and would be inconsistent with Eq. (101), which is based upon an assumption that B is continuous.

The present formulation closely resembles that of Ref. 1, differing chiefly in that opacities are evaluated at interfaces rather than at zone midpoints. This variation is intended to facilitate a more versatile treatment of radiation front propagation with little or no accompanying increase in computation.

The cross section σ, considered as a function of ν, or of $u = h\nu/\theta$, has too detailed a structure to permit approximation in one stage to be a practical procedure. Subintervals Δu_k are therefore defined which are sufficiently small so that within them the variations of the Planck and Rosseland spectrum functions, $W_1(u)$ and $W_2(u)$, are negligible. The opacity within these subintervals may or may not show considerable variation. In any case, it can be at least partially described by the direct and inverse means (Ref. 3)

$$\sigma_k^d = \int_{\Delta u_k} \sigma(u)du/\Delta u_k \tag{103}$$

$$\sigma_k^i = \Delta u_k / \int_{\Delta u_k} du/\sigma(u) \tag{104}$$

which are in effect microscopic Planck and Rosseland means, respectively.

The number of these subintervals is, typically, of order 10^2 to 10^4. The number of groups employed in transport calculations, however, is of order 1 to 10^2. It is not generally possible to neglect the variation of $W_1(u)$ and $W_2(u)$ within these groups. Thus, for the subintervals Δu_k contained within a group $u_j \leq u < u_{j+1}$, one defines normalized Planck and Rosseland weights:

$$P_k = \frac{f(u_k) - f(u_k + \Delta u_k)}{f(u_j) - f(u_{j+1})} \tag{105}$$

$$R_k = \frac{[f(u_k) - f(u_k + \Delta u_k) + g(u_k) - g(u_k + \Delta u_k)] / \sigma_k^i}{\sum_\ell [f(u_\ell) - f(u_\ell + \Delta u_\ell) + g(u_\ell) - g(u_\ell + \Delta u_\ell)] / \sigma_\ell^i} \tag{106}$$

The group Planck and Rosseland cross sections and transmission functions are thus, respectively,

$$\sigma_{ij}^{P} = \sum_{k} P_k \sigma_k^d \tag{107}$$

$$\sigma_{ij}^{R} = \sum_{k} R_k \sigma_k^i \tag{108}$$

$$S_{ij}(x) = \sum_{k} P_k e^{-\sigma_k^d x} \tag{109}$$

$$T_{ij}(x) = \sum_{k} R_k e^{-\sigma_k^i x} \tag{110}$$

These are the discrete analogs of Eqs. (93) through (96). Although Eqs. (107) and (108) are essentially exact, Eqs. (109) and (110) are already approximations which are accurate only to first order in x. Even so, they are still far too cumbersome for use by the transport routines, which require representations $\bar{S}_{ij}(x)$ and $\bar{T}_{ij}(x)$ of $S_{ij}(x)$ and $T_{ij}(x)$ involving at most five or six parameters each, with the use of exponential or similar functions kept to a minimum. On the other hand, the optical thickness of zones employed in transport calculations is unrestricted, so that the parameterization must not fail in a gross manner for any nonnegative x.

6.3 PARAMETRIC REPRESENTATION OF TRANSMISSION FUNCTIONS

The method to be described employs piecewise-linear, and linear rational approximations to the logarithm of the transmission function. Both functions (109) and (110) are of the form

$$F(x) = \sum_{k} Q_k e^{-\sigma_k x} \tag{111}$$

with

$$F(0) = \sum_{k} Q_k = 1 \tag{112}$$

In accordance with Eq. (107) or (108), define

$$-F'(0) = \sum_k Q_k \sigma_k = \bar{\sigma} \tag{113}$$

The (Planck or Rosseland) optical depth variable is then

$$\tau = \bar{\sigma} x \tag{114}$$

Let

$$\overline{\sigma^2} = \sum_k Q_k \sigma_k^2 \tag{115}$$

Then the expansion of (111) in powers of τ is

$$F(x) = F(\tau) = 1 - \tau + 1/2 \frac{\overline{\sigma^2}}{\bar{\sigma}^2} \tau^2 - \ldots \tag{116}$$

The approximation

$$\bar{F}(\tau) = e^{-\tau \bar{H}(\tau)} \tag{117}$$

with

$$\bar{H}(\tau) = 1 - \frac{\overline{\sigma^2} - \bar{\sigma}^2}{2\bar{\sigma}^2} \tau, \qquad 0 \le \tau < \tau_1 \tag{118}$$

agrees with Eq. (116) to second order in τ. For τ not small compared with unity, this approximation can be very poor. The general linear fit is therefore used:

$$\bar{H}(\tau) = \bar{H}(\tau_2) + \frac{H(\tau_3) - H(\tau_2)}{\tau_3 - \tau_2}(\tau - \tau_2), \qquad \tau_1 \le \tau < \tau_3 \tag{119}$$

where τ_1 is the abscissa of the intersection of the two lines (118) and (119), τ_2 and τ_3 are prescribed values such as

$$\tau_2 = \bar{\sigma}/\sigma^P, \qquad \tau_3 = \bar{\sigma}/\sigma^R \tag{120}$$

and

$$H(\tau_2) = -\ln F(\tau_2)/\tau_2, \qquad H(\tau_3) = -\ln F(\tau_3)/\tau_3 \tag{121}$$

(It is assumed that $\sigma^P > \sigma^R$ so that $\tau_3 > \tau_2$. If scattering is included in σ^R but not in σ^P, this condition may not be satisfied and a different prescription of τ_2 and τ_3 should be used). Finally, for $\tau \to \infty$ the approximation used is the linear rational function

$$\bar{H}(\tau) = \frac{b_1 + b_2\tau}{b_3 + b_4\tau} \qquad \tau_3 \leq \tau < \infty \tag{122}$$

where
$$\begin{aligned}
b_1 &= H(\tau_3)H(\tau_4)\tau_4(\tau_4 - \tau_3) + H(\tau_4)\tau_3 - H(\tau_3)\tau_4 \\
b_2 &= H(\tau_3) - H(\tau_4) \\
b_3 &= \tau_3 + \tau_4[H(\tau_4)\tau_4 - H(\tau_3)\tau_3 - 1] \\
b_4 &= \tau_4 b_2 \\
\tau_4 &= \frac{\bar{\sigma}}{\min(\sigma_k)} \\
H(\tau_4) &= -\ln F(\tau_4)/\tau_4
\end{aligned}$$

This function has the properties

$$\begin{aligned}
\bar{H}(\tau_3) &= H(\tau_3) \\
\bar{H}(\tau_4) &= H(\tau_4)
\end{aligned}$$

and $\lim_{\tau\to\infty} \bar{\sigma}\,\bar{H}(\tau) = \lim_{\tau\to\infty} \bar{\sigma}\,H(\tau) = \min(\sigma_k)$, where $\min(\sigma_k)$ is the smallest of all the σ_k^d or σ_k^i in the group.

The parameterization described requires storage of 12 parameters on a "DIANE"-type data file for use by the radiation transport routines; for example; σ^P, σ^R, $\min(\sigma_k^d)$, $\min(\sigma_k^i)$, τ_1^P, τ_1^R, $H^P(\tau_1)$, $H^R(\tau_1)$, $H^P(\tau_3)$, $H^R(\tau_3)$, $H^P(\tau_4)$, and $H^R(\tau_4)$. The accuracy of fit attainable with these parameters has been investigated for a few artifical examples. The poorest fit generally occurs in the S function for cases in which $\sigma^P \gg \sigma^R$, for widths $\delta = x$ such that

$$\frac{1}{\sigma^P} \ll x \ll \frac{1}{\sigma^R}$$

In extreme cases of this type the fit is still usually within a factor of two. If σ^P and σ^R are within one or two orders of magnitude, the worst fit is of the order of 10%. For depths small compared with a mean free path, the fit is generally excellent, although in the worst cases the T function may be in error by 10% or so near $\sigma^R = 0.5$. Since the difference between $\min(\sigma_k^d)$ and $\min(\sigma_k^i)$ is not significant except at very large depths, it would be possible to use a single value for both, reducing the required number of parameters to 11. Still fewer parameters could be used if the resulting loss of accuracy is considered acceptable.

A number of other parameterizations were explored, including fitting by sums of exponentials and various techniques using orthogonal polynomials and higher order rational approximants to the logarithm of the transmission function. Of those investigated, only the fit by a sum of exponentials appeared at all satisfactory, and the technique described above offers comparable results with much less computational time involved. Undoubtedly, the present parameterization can be further improved, but it is believed that this type of approach offers acceptable accuracy along with reasonable economy in the handling of data better than most others.

REFERENCES

1. Freeman, B. E., "Frequency-group Average Absorption Coefficients for SPUTTER," General Atomic Informal Report, GAMD-6446, June 1965.
2. Sampson, D. H., Radiative Contributions to Energy and Momentum Transport in a Gas, Interscience Publishers, New York, 1965, p. 102.
3. Stewart, John C., and K. D. Pyatt, Jr., "Theoretical Study of Optical Properties," Air Force Special Weapons Center Report AF SWC/TR/61-71, Vols. I, II, III, General Atomic Division, General Dynamics Corporation, September, 1961.

Unclassified

Security Classification

DOCUMENT CONTROL DATA - R&D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author) General Atomic Division General Dynamics Corporation San Diego, California	2a. REPORT SECURITY CLASSIFICATION Unclassified 2b GROUP

3. REPORT TITLE
NUCLEAR EXPLOSION INTERACTION STUDIES
VOLUME I: METHODS FOR ANALYSIS OF RADIATIVE TRANSFER

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)
Final Report 22 July 1965 to 21 July 1966

5. AUTHOR(S) (Last name, first name, initial)
Pyatt, K. D., Jr., et al.

6. REPORT DATE May 1967	7a. TOTAL NO. OF PAGES 158	7b. NO. OF REFS 30

8a. CONTRACT OR GRANT NO. AF29(601)-7035 b. PROJECT NO. 5710 c. Subtask No. 07.002 d.	9a. ORIGINATOR'S REPORT NUMBER(S) AFWL-TR-66-108, Vol. I 9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report) Contractor's Report No. GA-7370

10. AVAILABILITY/LIMITATION NOTICES This document is subject to special export controls and each transmittal to foreign governments or foreign nationals may be made only with prior approval of AFWL (WLRT), Kirtland AFB, N.M. Distribution of this document is limited because of the technology discussed.

11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY Air Force Weapons Laboratory (WLRT) Kirtland Air Force Base, New Mexico 87117

13. ABSTRACT

The non-equilibrium diffusion approximation to the radiative-transfer equation is developed. The first two moments of the radiative transfer equation, including Thomson scattering and pure absorption, are formed, and the equations are closed by a relation between the radiation energy and pressure. Applications of SPUTTER non-equilibrium diffusion subroutines to several simple radiative-transfer problems are described and compared with results from other numerical radiative-transfer codes. Subroutines are also described which calculate the effect of Thomson scattering in TAMALE. The method of moments, the method of discrete ordinates or characteristics, and the Monte Carlo method are described with special reference to the calculation of radiative transport in two dimensions. Their relative merits are discussed, and considerations bearing on the choice of which to use in various applications are given. The non-equilibrium diffusion approximation, which is the variant of the moments method used in DRADTN and ERADTN, has been extended to axially symmetric configurations of two dimensions in a new program, TDRAD. The method of characteristics has been programmed for the same geometry as that treated by TDRAD. The new code, TRAN2, extends TDRAD to situations in which the radiation is too anisotropic to be described by only two moments. The problem of averaging absorption coefficients and scattering cross sections is a basic one in any calculation of radiative transport. A proposed solution is formulated, and transmission functions are derived for the case where opacities may be considered piecewise constant in space and frequency.

(Distribution Limitation Statement No. 2)

DD FORM 1 JAN 64 1473

Unclassified

Security Classification

Unclassified

Security Classification

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Radiation transport						
One-dimensional hydrodynamics						
Nonequilibrium diffusion						
Compton scattering						
Thomson scattering						
Two-dimensional radiation transport						

INSTRUCTIONS

1. **ORIGINATING ACTIVITY:** Enter the name and address of the contractor, subcontractor, grantee, Department of Defense activity or other organization *(corporate author)* issuing the report.

2a. **REPORT SECURITY CLASSIFICATION:** Enter the overall security classification of the report. Indicate whether "Restricted Data" is included. Marking is to be in accordance with appropriate security regulations.

2b. **GROUP:** Automatic downgrading is specified in DoD Directive 5200.10 and Armed Forces Industrial Manual. Enter the group number. Also, when applicable, show that optional markings have been used for Group 3 and Group 4 as authorized.

3. **REPORT TITLE:** Enter the complete report title in all capital letters. Titles in all cases should be unclassified. If a meaningful title cannot be selected without classification, show title classification in all capitals in parenthesis immediately following the title.

4. **DESCRIPTIVE NOTES:** If appropriate, enter the type of report, e.g., interim, progress, summary, annual, or final. Give the inclusive dates when a specific reporting period is covered.

5. **AUTHOR(S):** Enter the name(s) of author(s) as shown on or in the report. Enter last name, first name, middle initial. If military, show rank and branch of service. The name of the principal author is an absolute minimum requirement.

6. **REPORT DATE:** Enter the date of the report as day, month, year; or month, year. If more than one date appears on the report, use date of publication.

7a. **TOTAL NUMBER OF PAGES:** The total page count should follow normal pagination procedures, i.e., enter the number of pages containing information.

7b. **NUMBER OF REFERENCES:** Enter the total number of references cited in the report.

8a. **CONTRACT OR GRANT NUMBER:** If appropriate, enter the applicable number of the contract or grant under which the report was written.

8b, 8c, & 8d. **PROJECT NUMBER:** Enter the appropriate military department identification, such as project number, subproject number, system numbers, task number, etc.

9a. **ORIGINATOR'S REPORT NUMBER(S):** Enter the official report number by which the document will be identified and controlled by the originating activity. This number must be unique to this report.

9b. **OTHER REPORT NUMBER(S):** If the report has been assigned any other report numbers *(either by the originator or by the sponsor)*, also enter this number(s).

10. **AVAILABILITY/LIMITATION NOTICES:** Enter any limitations on further dissemination of the report, other than those imposed by security classification, using standard statements such as:

(1) "Qualified requesters may obtain copies of this report from DDC."

(2) "Foreign announcement and dissemination of this report by DDC is not authorized."

(3) "U. S. Government agencies may obtain copies of this report directly from DDC. Other qualified DDC users shall request through ________________."

(4) "U. S. military agencies may obtain copies of this report directly from DDC. Other qualified users shall request through ________________."

(5) "All distribution of this report is controlled. Qualified DDC users shall request through ________________."

If the report has been furnished to the Office of Technical Services, Department of Commerce, for sale to the public, indicate this fact and enter the price, if known.

11. **SUPPLEMENTARY NOTES:** Use for additional explanatory notes.

12. **SPONSORING MILITARY ACTIVITY:** Enter the name of the departmental project office or laboratory sponsoring *(paying for)* the research and development. Include address.

13. **ABSTRACT:** Enter an abstract giving a brief and factual summary of the document indicative of the report, even though it may also appear elsewhere in the body of the technical report. If additional space is required, a continuation sheet shall be attached.

It is highly desirable that the abstract of classified reports be unclassified. Each paragraph of the abstract shall end with an indication of the military security classification of the information in the paragraph, represented as *(TS)*, *(S)*, *(C)*, or *(U)*.

There is no limitation on the length of the abstract. However, the suggested length is from 150 to 225 words.

14. **KEY WORDS:** Key words are technically meaningful terms or short phrases that characterize a report and may be used as index entries for cataloging the report. Key words must be selected so that no security classification is required. Identifiers, such as equipment model designation, trade name, military project code name, geographic location, may be used as key words but will be followed by an indication of technical context. The assignment of links, rules, and weights is optional.